

Appendix A

Mathematical Symbols and Notation

A.1 Symbols

The following symbols are used in the main text primarily with the denotations given here. While some symbols may be used for purposes other than the ones listed, the meaning should always be clear in the particular context.

(a_0, \dots, a_{n-1}) A *vector* or *list*, that is, an ordered sequence of n elements of the same type. Unlike a *set* (see below), a list may contain the same element more than once. If used to denote a *vector*, then (a_0, \dots, a_{n-1}) is usually a *row* vector and $(a_0, \dots, a_{n-1})^\top$ is the corresponding (transposed) *column* vector.¹ If used to represent a *list*,² $()$ represents the *empty* list and (a) is a list with a single element a . $|A|$ is the *length* of the sequence A , that is, the number of contained elements. $A \sim B$ denotes the concatenation of A, B . $A(i)$ or a_i refers to the i -th element of A . $A(i) \leftarrow x$ means that the i -th element of A is set to (i.e., replaced by) the quantity x .

$\{a, b, c, d, \dots\}$ A *set*, that is, an unordered collection of distinct elements. A particular element x can be contained in a set at most once. $\{\}$ denotes the empty set. $|\mathcal{A}|$ is the size (cardinality) of the set \mathcal{A} . $\mathcal{A} \cup \mathcal{B}$ is the union and $\mathcal{A} \cap \mathcal{B}$ is the intersection of two sets \mathcal{A}, \mathcal{B} . $x \in \mathcal{A}$ means that the element x is contained in \mathcal{A} .

$\langle A, B, C \rangle$ A *tuple*, that is, a fixed-size, ordered sequence of elements, each possibly of a different type.³

¹ In most programming environments, vectors are implemented as one-dimensional arrays, with elements being referred to by position (index).

² Lists are usually implemented with dynamic data structures, such as linked lists. Java's *Collections* framework provides numerous easy-to-use list implementations.

³ Tuples are typically implemented as *objects* (in Java or C++) or *structures* (in C) with elements being referred to by name.

$[a, b]$	Numeric interval; $x \in [a, b]$ means $a \leq x \leq b$. Similarly, $x \in]a, b[$ says that $a < x < b$.
$ A $	Length (number of elements) of a sequence (see above) or size (cardinality) of a set A , that is, $ A \equiv \text{card } A$.
$ \mathbf{A} $	Determinant of a matrix \mathbf{A} ($ \mathbf{A} \equiv \det(\mathbf{A})$).
$ x $	Absolute value (magnitude) of a scalar or complex quantity x .
$\ \mathbf{x}\ $	Euclidean (L_2) norm of a vector \mathbf{x} . $\ \mathbf{x}\ _n$ denotes the magnitude of \mathbf{x} using a particular norm L_n .
$\lceil x \rceil$	“Ceil” of x , the smallest integer $z \in \mathbb{Z}$ greater than $x \in \mathbb{R}$. For example, $\lceil 3.141 \rceil = 4$, $\lceil -1.2 \rceil = -1$.
$\lfloor x \rfloor$	“Floor” of x , the largest integer $z \in \mathbb{Z}$ smaller than $x \in \mathbb{R}$. For example, $\lfloor 3.141 \rfloor = 3$, $\lfloor -1.2 \rfloor = -2$.
\div	Integer division operator: $a \div b$ denotes the quotient of the two integers a, b . For example, $5 \div 3 = 1$ and $-13 \div 4 = -3$ (equivalent to Java’s “/” operator in the case of integer operands).
$*$	Linear convolution operator (see Sec. 5.3.1).
\otimes	Linear correlation operator (see Sec. 23.1.1).
\otimes	Outer vector product (see Sec. B.3.2).
\times	Cross product (between vectors or complex quantities (see Sec. B.3.3)).
\oplus	Morphological dilation operator (see Sec. 9.2.3).
\ominus	Morphological erosion operator (see Sec. 9.2.4).
\circ	Morphological opening operator (see Sec. 9.3.1).
\bullet	Morphological closing operator (see Sec. 9.3.2).
\smile	Concatenation operator. Given two sequences $A = (a, b, c)$ and $B = (d, e)$, $A \smile B$ denotes the concatenation of A and B , with the result (a, b, c, d, e) . Inserting a single element x at the end or front of the list A is written as $A \smile (x)$ or $(x) \smile A$, resulting in (a, b, c, x) or (x, a, b, c) , respectively.
\sim	“Similarity” relation used in the context of random variables and statistical distributions.
\approx	“Approximately equal” relation.
\equiv	Equivalence relation.
\leftarrow	Assignment operator: $a \leftarrow expr$ means that expression $expr$ is evaluated and subsequently the result is assigned to the variable a .
\leftarrow^{\pm}	Incremental assignment operator: $a \leftarrow^{\pm} b$ is equivalent to $a \leftarrow a \pm b$.
$:=$	Function definition operator (used in algorithms). For example, $f(x) := x^2 + 5$ defines a function $f()$ with the bound variable (formal function argument) x .
\dots	“upto” (incrementing) iteration, used in loop constructs like for $q \leftarrow 1, \dots, K$ (with $q = 1, 2, \dots, K-1, K$).
\dots	“downto” (decrementing) iteration, for example, for $q \leftarrow K, \dots, 1$ (with $q = K, K-1, \dots, 2, 1$).

- \wedge Logical “and” operator.
- \vee Logical “or” operator.
- ∂ Partial derivative operator (see Sec. 6.2.1). For example, $\frac{\partial}{\partial x_i} f$ denotes the *first* derivative of the multi-dimensional function $f(x_1, x_2, \dots, x_n) : \mathbb{R}^n \rightarrow \mathbb{R}$ along variable x_i , $\frac{\partial^2}{\partial x_i^2} f$ is the *second* derivative (i.e., differentiating f twice along variable x_i), etc.
- ∇ Gradient operator. The gradient of a multi-dimensional function $f(x_1, x_2, \dots, x_n) : \mathbb{R}^n \rightarrow \mathbb{R}$, denoted ∇f (also ∇_f or $\text{grad } f$), is the vector of its first partial derivatives (see also Sec. C.2.2).
- ∇^2 Laplace operator (or *Laplacian*). The Laplacian of a multi-dimensional function $f(x_1, x_2, \dots, x_n) : \mathbb{R}^n \rightarrow \mathbb{R}$, denoted $\nabla^2 f$ (or ∇_f^2), is the sum of its second partial derivatives (see Sec. C.2.5).
- $\mathbf{0}$ Zero vector, $\mathbf{0} = (0, \dots, 0)^\top$.
- adj Adjugate of a square matrix, denoted $\text{adj}(\mathbf{A})$; also called *adjoint* in older texts.
- AND Bitwise “and” operation. Example: $(0011_{\text{b}} \text{ AND } 1010_{\text{b}}) = 0010_{\text{b}}$ (binary) and $(3 \text{ AND } 6) = 2$ (decimal).
- ArcTan(x, y) Inverse tangent function. The result of $\text{ArcTan}(x, y)$ is equivalent to $\arctan(\frac{y}{x}) = \tan^{-1}(\frac{y}{x})$ but with two arguments and returning angles in the range $[-\pi, +\pi]$ (i.e., covering all four quadrants). $\text{ArcTan}(x, y)$ is equivalent to the $\text{ArcTan}[\mathbf{x}, \mathbf{y}]$ function in *Mathematica* and the $\text{Math.atan2}(y, x)$ method in Java (but note the reversed arguments!).
- \mathbb{C} The set of complex numbers.
- card Size (cardinality) of a set. $\text{card}(\mathcal{A}) = |\mathcal{A}|$ (see also Sec. 3.1).
- det Determinant of a matrix ($\det(\mathbf{A}) = |\mathbf{A}|$).
- DFT Discrete Fourier transform (see Sec. 18.3).
- e Euler’s constant.
- \mathbf{e} Unit vector. For example, $\mathbf{e}_x = (1, 0)^\top$ denotes the 2D unit vector in x -direction. $\mathbf{e}_\theta = (\cos \theta, \sin \theta)^\top$ is the 2D unit vector oriented at angle θ and $\mathbf{e}_i, \mathbf{e}_j, \mathbf{e}_k$ are the unit vectors along the coordinate axes in 3D.
- exp Exponential function: $\exp(x) = e^x$.
- \mathcal{F} Continuous Fourier transform (see Sec. 18.1.4).
- false Boolean constant (false = \neg true).
- grad Gradient operator (see ∇).
- h Histogram of an image (see Sec. 3.1).
- H Cumulative histogram (see Sec. 3.6).
- \mathbf{H} Hessian matrix (see Sec. C.2.6).
- hom Operator for converting Cartesian to homogeneous coordinates. $\text{hom}(\mathbf{x}) = \underline{\mathbf{x}}$ maps the Cartesian point \mathbf{x} to a corresponding homogeneous point $\underline{\mathbf{x}}$; the reverse mapping is denoted $\text{hom}^{-1}(\underline{\mathbf{x}}) = \mathbf{x}$ (see Sec. B.5).
- i Imaginary unit ($i^2 = -1$), see Sec. A.3.

I	Image with scalar pixel values (e.g., an intensity or grayscale image). $I(u, v) \in \mathbb{R}$ is the pixel value at position (u, v)
\mathbf{I}	Vector-valued image, for example, a RGB color image with 3D color vectors $\mathbf{I}(u, v) \in \mathbb{R}^3$ at position (u, v) .
\mathbf{I}_n	Identity matrix of size $n \times n$. For example, $\mathbf{I}_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ is the 2×2 identity matrix.
\mathbf{J}	Jacobian matrix (see Sec. C.2.1).
L_1, L_2, L_∞	Common distance measures or <i>norms</i> (see Eqns. (15.23)–(15.25)).
$M \times N$	Domain of pixel coordinates (u, v) for an image with M columns (width) and N rows (height); used as a shortcut notation for the set $\{0, \dots, M-1\} \times \{0, \dots, N-1\}$.
mod	Modulus operator: $(a \bmod b)$ is the remainder of the <i>integer</i> division $a \div b$ (see Sec. F.1.2).
μ	Arithmetic mean value.
\mathbb{N}	The set of natural numbers; $\mathbb{N} = \{1, 2, 3, \dots\}$, $\mathbb{N}_0 = \{0, 1, 2, \dots\}$.
nil	Null (“nothing”) constant, typically used in algorithms to denote an invalid quantity (similar to <code>null</code> in Java).
p	Discrete probability density function (see Sec. 4.6.1).
P	Discrete probability distribution function or cumulative probability density (see Sec. 4.6.1).
\mathcal{Q}	Quadrilateral (see Sec. 21.1.4).
\mathbb{R}	The set of real numbers.
R, G, B	<i>Red, green and blue</i> color components.
rank	Rank of a matrix \mathbf{A} , denoted by $\text{rank}(\mathbf{A})$.
round	Rounding function: returns the integer closest to the scalar $x \in \mathbb{R}$. $\text{round}(x) \equiv \lfloor x + 0.5 \rfloor$.
σ	Standard deviation (square root of the <i>variance</i> σ^2).
\mathcal{S}_1	Unit square (see Sec. 21.1.4).
sgn	“Sign” or “signum” function: $\text{sgn}(x) = \begin{cases} 1 & \text{for } x > 0 \\ 0 & \text{for } x = 0 \\ -1 & \text{for } x < 0 \end{cases}$
τ	Interval in time or space.
t	Continuous time variable.
t	Threshold value.
\top	Transpose of a vector (\mathbf{a}^\top) or matrix (\mathbf{A}^\top).
trace	Trace (sum of the diagonal elements) of a matrix, e.g., $\text{trace}(\mathbf{A})$.
true	Boolean constant (true = \neg false).
$\mathbf{u} = (u, v)$	Discrete 2D coordinate variable with $u, v \in \mathbb{Z}$.
$\mathbf{x} = (x, y)$	Continuous 2D coordinate variable with $x, y \in \mathbb{R}$.
XOR	Bitwise “xor” (exclusive OR) operator. Example: $(0011_{\text{b}} \text{ XOR } 1010_{\text{b}}) = 1001_{\text{b}}$ (binary) and $(3 \text{ XOR } 6) = 5$ (decimal).
\mathbb{Z}	The set of integers.

A.2 Set Operators

- $|\mathcal{A}|$ The size of the set \mathcal{A} (equal to $\text{card}(\mathcal{A})$).
 $\forall_x \dots$ “All” quantifier (for all x, \dots).
 $\exists_x \dots$ “Exists” quantifier (there is some x for which \dots).
 \cup Set union (e.g., $\mathcal{A} \cup \mathcal{B}$).
 \cap Set intersection (e.g., $\mathcal{A} \cap \mathcal{B}$).
 $\bigcup_i \mathcal{A}_i$ Union of multiple sets \mathcal{A}_i .
 $\bigcap_i \mathcal{A}_i$ Intersection over multiple sets \mathcal{A}_i .
 \setminus Set difference: if $x \in \mathcal{A} \setminus \mathcal{B}$, then $x \in \mathcal{A}$ and $x \notin \mathcal{B}$.

A.3 Complex Numbers

Basic relations:

$$z = a + i \cdot b \quad (\text{with } z, i \in \mathbb{C}, a, b \in \mathbb{R}, i^2 = -1) \quad (\text{A.1})$$

$$s \cdot z = s \cdot a + i \cdot s \cdot b \quad (\text{for } s \in \mathbb{R}) \quad (\text{A.2})$$

$$|z| = \sqrt{a^2 + b^2} \quad (\text{A.3})$$

$$|s \cdot z| = s \cdot |z| \quad (\text{A.4})$$

$$z = a + i \cdot b = |z| \cdot (\cos \psi + i \cdot \sin \psi) \quad (\text{A.5})$$

$$= |z| \cdot e^{i \cdot \psi} \quad (\text{with } \psi = \text{ArcTan}(a, b)) \quad (\text{A.6})$$

$$\text{Re}(a + i \cdot b) = a \quad \text{Re}(e^{i \cdot \varphi}) = \cos \varphi \quad (\text{A.7})$$

$$\text{Im}(a + i \cdot b) = b \quad \text{Im}(e^{i \cdot \varphi}) = \sin \varphi \quad (\text{A.8})$$

$$e^{i \cdot \varphi} = \cos \varphi + i \cdot \sin \varphi \quad (\text{A.9})$$

$$e^{-i \cdot \varphi} = \cos \varphi - i \cdot \sin \varphi \quad (\text{A.10})$$

$$\cos(\varphi) = \frac{1}{2} \cdot (e^{i \cdot \varphi} + e^{-i \cdot \varphi}) \quad (\text{A.11})$$

$$\sin(\varphi) = \frac{1}{2i} \cdot (e^{i \cdot \varphi} - e^{-i \cdot \varphi}) \quad (\text{A.12})$$

$$z^* = a - i \cdot b \quad (\text{complex conjugate}) \quad (\text{A.13})$$

$$z \cdot z^* = z^* \cdot z = |z|^2 = a^2 + b^2 \quad (\text{A.14})$$

$$z^0 = (a + i \cdot b)^0 = (1 + i \cdot 0) = 1 \quad (\text{A.15})$$

Arithmetic operations:

$$z_1 = (a_1 + i \cdot b_1) = |z_1| e^{i \cdot \varphi_1} \quad (\text{A.16})$$

$$z_2 = (a_2 + i \cdot b_2) = |z_2| e^{i \cdot \varphi_2} \quad (\text{A.17})$$

$$z_1 + z_2 = (a_1 + a_2) + i \cdot (b_1 + b_2), \quad (\text{A.18})$$

$$z_1 \cdot z_2 = (a_1 \cdot a_2 - b_1 \cdot b_2) + i \cdot (a_1 \cdot b_2 + b_1 \cdot a_2) \quad (\text{A.19})$$

$$= |z_1| \cdot |z_2| \cdot e^{i \cdot (\varphi_1 + \varphi_2)} \quad (\text{A.20})$$

$$\frac{z_1}{z_2} = \frac{a_1 \cdot a_2 + b_1 \cdot b_2}{a_2^2 + b_2^2} + i \cdot \frac{a_2 \cdot b_1 - a_1 \cdot b_2}{a_2^2 + b_2^2} = \frac{|z_1|}{|z_2|} \cdot e^{i \cdot (\varphi_1 - \varphi_2)} \quad (\text{A.21})$$

Appendix B

Linear Algebra

This part contains a compact set of elementary tools and concepts from algebra and calculus that are referenced in the main text. Many good textbooks (probably including some of your school books) are available on this subject, for example, [35,36,145,264]. For numerical aspects of linear algebra see [160,190].

B.1 Vectors and Matrices

Here we describe the basic notation for vectors in two and three dimensions. Let

$$\mathbf{a} = \begin{pmatrix} a_0 \\ a_1 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} b_0 \\ b_1 \end{pmatrix} \quad (\text{B.1})$$

denote vectors \mathbf{a}, \mathbf{b} in 2D, and analogously

$$\mathbf{a} = \begin{pmatrix} a_0 \\ a_1 \\ a_2 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} b_0 \\ b_1 \\ b_2 \end{pmatrix} \quad (\text{B.2})$$

vectors in 3D (with $a_i, b_i \in \mathbb{R}$). Vectors are used to describe 2D or 3D points (relative to the origin of the coordinate system) or the displacement between two arbitrary points in the corresponding space.

We commonly use upper-case letters to denote a *matrix*, for example,

$$\mathbf{A} = \begin{pmatrix} A_{0,0} & A_{0,1} \\ A_{1,0} & A_{1,1} \\ A_{2,0} & A_{2,1} \end{pmatrix}. \quad (\text{B.3})$$

This matrix consists of 3 rows and 2 columns; in other words, \mathbf{A} is of size $(3, 2)$. Its individual elements are referenced as $A_{i,j}$, where i is the *row* index (vertical coordinate) and j is the *column* index (horizontal coordinate).¹

¹ Note that the usual notation for matrix coordinates is (unlike image coordinates) vertical-first!

The *transpose* of \mathbf{A} , denoted \mathbf{A}^\top , is obtained by exchanging rows and columns, that is,

$$\mathbf{A}^\top = \begin{pmatrix} A_{0,0} & A_{0,1} \\ A_{1,0} & A_{1,1} \\ A_{2,0} & A_{2,1} \end{pmatrix}^\top = \begin{pmatrix} A_{0,0} & A_{1,0} & A_{2,0} \\ A_{0,1} & A_{1,1} & A_{2,1} \end{pmatrix}. \quad (\text{B.4})$$

The *inverse* of a square matrix \mathbf{A} is denoted \mathbf{A}^{-1} , such that

$$\mathbf{A} \cdot \mathbf{A}^{-1} = \mathbf{I} \quad \text{and} \quad \mathbf{A}^{-1} \cdot \mathbf{A} = \mathbf{I} \quad (\text{B.5})$$

(\mathbf{I} is the identity matrix). Note that not every square matrix has an inverse. Calculation of the inverse can be performed in closed form up to the size (3, 3); for example, see Eqn. (21.29) and Eqn. (24.47). In general, the use of standard numerical methods is recommended (see Sec. B.6).

B.1.1 Column and Row Vectors

For practical purposes, a vector can be considered a special case of a matrix. In particular, a the m -dimensional *column* vector

$$\mathbf{a} = \begin{pmatrix} a_0 \\ \vdots \\ a_{m-1} \end{pmatrix} \quad (\text{B.6})$$

corresponds to a matrix of size $(m, 1)$, while its transpose \mathbf{a}^\top is a *row* vector and thus like a matrix of size $(1, m)$. By default, and unless otherwise noted, any vector is implicitly assumed to be a *column* vector.

B.1.2 Length (Norm) of a Vector

The *length* or *Euclidean norm* (L_2 norm) of a vector $\mathbf{a} = (a_1, \dots, a_{m-1})^\top$, denoted $\|\mathbf{a}\|$, is defined as

$$\|\mathbf{a}\| = \left(\sum_{i=0}^{m-1} a_i^2 \right)^{1/2}. \quad (\text{B.7})$$

For example, the length of the 3D vector $\mathbf{x} = (x, y, z)^\top$ is

$$\|\mathbf{x}\| = \sqrt{x^2 + y^2 + z^2}. \quad (\text{B.8})$$

B.2 Matrix Multiplication

B.2.1 Scalar Multiplication

The product of a real-valued matrix and a scalar value $s \in \mathbb{R}$ is defined as

$$s \cdot \mathbf{A} = \mathbf{A} \cdot s = [s \cdot A_{i,j}] = \begin{pmatrix} s \cdot A_{0,0} & \cdots & s \cdot A_{0,n-1} \\ \vdots & \ddots & \vdots \\ s \cdot A_{m-1,0} & \cdots & s \cdot A_{m-1,n-1} \end{pmatrix}. \quad (\text{B.9})$$

B.2.2 Product of Two Matrices

We say that a matrix is of size (m, n) if consists of m rows and n columns. Given two matrices \mathbf{A} , \mathbf{B} of size (m, n) and (p, q) , respectively, the product $\mathbf{A} \cdot \mathbf{B}$ is only defined if $n = p$. Thus the number of columns (n) in \mathbf{A} must always match the number of rows (p) in \mathbf{B} . The result is a new matrix \mathbf{C} of size (m, q) , that is,

$$\begin{aligned} \mathbf{C} = \mathbf{A} \cdot \mathbf{B} &= \underbrace{\begin{pmatrix} A_{0,0} & \cdots & A_{0,n-1} \\ \vdots & \ddots & \vdots \\ A_{m-1,0} & \cdots & A_{m-1,n-1} \end{pmatrix}}_{(m,n)} \cdot \underbrace{\begin{pmatrix} B_{0,0} & \cdots & B_{0,q-1} \\ \vdots & \ddots & \vdots \\ B_{n-1,0} & \cdots & B_{n-1,q-1} \end{pmatrix}}_{(n,q)} \\ &= \underbrace{\begin{pmatrix} C_{0,0} & \cdots & C_{0,q-1} \\ \vdots & \ddots & \vdots \\ C_{m-1,0} & \cdots & C_{m-1,q-1} \end{pmatrix}}_{(m,q)}, \end{aligned} \quad (\text{B.10})$$

with the elements

$$C_{ij} = \sum_{k=0}^{n-1} A_{i,k} \cdot B_{k,j}, \quad (\text{B.11})$$

for $i = 0, \dots, m-1$ and $j = 0, \dots, q-1$. Note that this product is not commutative, that is, $\mathbf{A} \cdot \mathbf{B} \neq \mathbf{B} \cdot \mathbf{A}$ in general.

B.2.3 Matrix-Vector Products

The product $\mathbf{A} \cdot \mathbf{x}$ between a matrix \mathbf{A} and a vector \mathbf{x} is only a special case of the matrix-matrix multiplication given in Eqn. (B.10). In particular, if $\mathbf{x} = (x_0, \dots, x_{n-1})^\top$ is a n -dimensional *column* vector (i.e., a matrix of size $(n, 1)$), then the multiplication

$$\underbrace{\mathbf{y}}_{(m,1)} = \underbrace{\mathbf{A}}_{(m,n)} \cdot \underbrace{\mathbf{x}}_{(n,1)} \quad (\text{B.12})$$

is only defined if the matrix \mathbf{A} is of size (m, n) , for arbitrary $m \geq 1$. The result \mathbf{y} is a *column* vector of length m (equivalent to a matrix of size $(m, 1)$). For example (with $m = 2$, $n = 3$),

$$\mathbf{A} \cdot \mathbf{x} = \underbrace{\begin{pmatrix} A & B & C \\ D & E & F \end{pmatrix}}_{(2,3)} \cdot \underbrace{\begin{pmatrix} x \\ y \\ z \end{pmatrix}}_{(3,1)} = \underbrace{\begin{pmatrix} A \cdot x + B \cdot y + C \cdot z \\ D \cdot x + E \cdot y + F \cdot z \end{pmatrix}}_{(2,1)}. \quad (\text{B.13})$$

Here \mathbf{A} operates on the column vector \mathbf{x} “from the left”, that is, $\mathbf{A} \cdot \mathbf{x}$ is the *left-sided* matrix-vector product of \mathbf{A} and \mathbf{x} .

Similarly, a *right-sided* multiplication of a *row* vector \mathbf{x}^\top of length m with a matrix of size (m, n) is performed as

$$\underbrace{\mathbf{x}^\top}_{(1,m)} \cdot \underbrace{\mathbf{B}}_{(m,n)} = \underbrace{\mathbf{z}}_{(1,n)}, \quad (\text{B.14})$$

where the result \mathbf{z} is a n -dimensional *row* vector; for example (again with $m = 2, n = 3$),

$$\mathbf{x}^\top \cdot \mathbf{B} = \underbrace{(x, y)}_{(1,2)} \cdot \underbrace{\begin{pmatrix} A & B & C \\ D & E & F \end{pmatrix}}_{(2,3)} = \underbrace{(x \cdot A + y \cdot D, x \cdot B + y \cdot E, x \cdot C + y \cdot F)}_{(1,3)}. \quad (\text{B.15})$$

In general, if $\mathbf{A} \cdot \mathbf{x}$ is defined, then

$$\mathbf{A} \cdot \mathbf{x} = (\mathbf{x}^\top \cdot \mathbf{A}^\top)^\top \quad \text{and} \quad (\mathbf{A} \cdot \mathbf{x})^\top = \mathbf{x}^\top \cdot \mathbf{A}^\top. \quad (\text{B.16})$$

Thus, any right-sided matrix-vector product $\mathbf{A} \cdot \mathbf{x}$ can also be calculated as a left-sided product $\mathbf{x}^\top \cdot \mathbf{A}^\top$ by transposing the corresponding matrix \mathbf{A} and vector \mathbf{x} .

B.3 Vector Products

Products between vectors are a common cause of confusion, mainly because the same symbol (\cdot) is used to denote widely different operators.

B.3.1 Dot (Scalar) Product

The *dot* product (also called *scalar* or *inner* product) of two vectors $\mathbf{a} = (a_0, \dots, a_{n-1})^\top$, $\mathbf{b} = (b_0, \dots, b_{n-1})^\top$ of the same length n is defined as

$$x = \mathbf{a} \cdot \mathbf{b} = \sum_{i=0}^{n-1} a_i \cdot b_i. \quad (\text{B.17})$$

Thus the result x is a scalar value (hence the name of this product). If we write this as the product of a row and a column vector, as in Eqn. (B.14),

$$\underbrace{x}_{(1,1)} = \underbrace{\mathbf{a}^\top}_{(1,n)} \cdot \underbrace{\mathbf{b}}_{(n,1)}, \quad (\text{B.18})$$

we conclude that the result x is a matrix of size $(1, 1)$, that is, a single scalar value. The dot product can be viewed as the *projection* of one vector onto the other, with the relation

$$\mathbf{a} \cdot \mathbf{b} = \|\mathbf{a}\| \cdot \|\mathbf{b}\| \cdot \cos(\alpha), \quad (\text{B.19})$$

where α is angle enclosed by the vectors \mathbf{a} and \mathbf{b} . As a consequence, the dot product is *zero* if the two vectors are *orthogonal* to each other.

The dot product of a vector with *itself* gives the square of its length (see Eqn. (B.7)), that is,

$$\mathbf{a} \cdot \mathbf{a} = \sum_{i=0}^{n-1} a_i^2 = \|\mathbf{a}\|^2. \quad (\text{B.20})$$

B.3.2 Outer Product

The outer product of two vectors $\mathbf{a} = (a_0, \dots, a_{m-1})^\top$, $\mathbf{b} = (b_0, \dots, b_{n-1})^\top$ of length m and n , respectively, is defined as

$$\mathbf{M} = \mathbf{a} \otimes \mathbf{b} = \mathbf{a} \cdot \mathbf{b}^\top = \begin{pmatrix} a_0 b_0 & a_0 b_1 & \dots & a_0 b_{n-1} \\ a_1 b_0 & a_1 b_1 & \dots & a_1 b_{n-1} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m-1} b_0 & a_{m-1} b_1 & \dots & a_{m-1} b_{n-1} \end{pmatrix}. \quad (\text{B.21})$$

Thus the result is a *matrix* \mathbf{M} with m rows and n columns and elements $M_{ij} = a_i \cdot b_j$, for $i = 0, \dots, m-1$ and $j = 1, \dots, n-1$. Note that $\mathbf{a} \cdot \mathbf{b}^\top$ in Eqn. (B.21) denotes the ordinary (matrix) product of the column vector \mathbf{a} (of size $m \times 1$) and the row vector \mathbf{b}^\top (of size $1 \times n$), as defined in Eqn. (B.10). The outer product is a special case of the *Kronecker* product (\otimes) which generally operates on pairs of matrices.

B.3.3 Cross Product

Although the cross product (\times) is generally defined for n -dimensional vectors, it is almost exclusively used in the 3D case, where the result is geometrically easy to understand. For a pair of 3D vectors, $\mathbf{a} = (a_0, a_1, a_2)^\top$ and $\mathbf{b} = (b_0, b_1, b_2)^\top$, the *cross product* is defined as

$$\mathbf{c} = \mathbf{a} \times \mathbf{b} = \begin{pmatrix} a_0 \\ a_1 \\ a_2 \end{pmatrix} \times \begin{pmatrix} b_0 \\ b_1 \\ b_2 \end{pmatrix} = \begin{pmatrix} a_1 \cdot b_2 - a_2 \cdot b_1 \\ a_2 \cdot b_0 - a_0 \cdot b_2 \\ a_0 \cdot b_1 - a_1 \cdot b_0 \end{pmatrix}. \quad (\text{B.22})$$

In the 3D case, the *cross product* is another 3D vector that is perpendicular to both of the original vectors.² The magnitude (length) of the vector \mathbf{c} relates to the angle θ between \mathbf{a} and \mathbf{b} as

$$\|\mathbf{c}\| = \|\mathbf{a} \times \mathbf{b}\| = \|\mathbf{a}\| \cdot \|\mathbf{b}\| \cdot \sin(\theta). \quad (\text{B.23})$$

The quantity $\|\mathbf{a} \times \mathbf{b}\|$ corresponds to the area of the parallelogram spanned by the vectors \mathbf{a} and \mathbf{b} .

B.4 Eigenvectors and Eigenvalues

This section gives an elementary introduction to eigenvectors and eigenvalues, which are mentioned at several places in the main text (see also [27, 64]). In general, the eigenvalue problem is to find solutions $\mathbf{x} \in \mathbb{R}^n$ and $\lambda \in \mathbb{R}$ for the linear equation

$$\mathbf{A} \cdot \mathbf{x} = \lambda \cdot \mathbf{x}, \quad (\text{B.24})$$

with the given square matrix \mathbf{A} of size (n, n) . Any non-trivial³ solution \mathbf{x} is an *eigenvector* of \mathbf{A} and the scalar λ (which may be

² For dimensions greater than three, the definition (and calculation) of the cross product is considerably more involved.

³ An obvious but trivial solution is $\mathbf{x} = \mathbf{0}$ (where $\mathbf{0}$ denotes the zero-vector).

complex-valued) is the associated *eigenvalue*. Eigenvalue and eigenvectors thus always come in pairs $\langle \lambda_j, \mathbf{x}_j \rangle$, usually called *eigenpairs*. Geometrically speaking, applying the matrix \mathbf{A} to an eigenvector only changes the vector's *magnitude* or *length* (by the associated eigenvalue λ), but not its orientation in space. Equation (B.24) can be rewritten as

$$\mathbf{A} \cdot \mathbf{x} - \lambda \cdot \mathbf{x} = \mathbf{0} \quad \text{or} \quad (\mathbf{A} - \lambda \cdot \mathbf{I}_n) \cdot \mathbf{x} = \mathbf{0}, \quad (\text{B.25})$$

where \mathbf{I}_n is the (n, n) identity matrix. This homogeneous linear equation has non-trivial solutions only if the matrix $(\mathbf{A} - \lambda \cdot \mathbf{I}_n)$ is *singular*, that is, its rank is *less* than n and thus its determinant $\det()$ is zero, that is,

$$\det(\mathbf{A} - \lambda \cdot \mathbf{I}_n) = 0. \quad (\text{B.26})$$

Equation (B.26) is called the “characteristic equation” of the matrix \mathbf{A} and can be expanded to a n -th order polynomial in λ . This polynomial has a maximum of n distinct roots, which are the eigenvalues of \mathbf{A} (that is, solutions to Eqn. (B.26)). A matrix of size (n, n) thus has up to n non-distinct eigenvectors $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$, each with an associated eigenvalue $\lambda_1, \lambda_2, \dots, \lambda_n$.

If they exist, the *eigenvalues* of a matrix are *unique*, but the associated *eigenvectors* are not! This results from the fact that, if Eqn. (B.24) is satisfied for a vector \mathbf{x} (and the associated eigenvalue λ), it also applies to any *scaled* vector $s\mathbf{x}$, that is,

$$\mathbf{A} \cdot s\mathbf{x} = \lambda \cdot s\mathbf{x}, \quad (\text{B.27})$$

for arbitrary $s \in \mathbb{R}$ (and $s \neq 0$). Thus, if \mathbf{x} is an eigenvector of \mathbf{A} , then $s\mathbf{x}$ is also an (equivalent) eigenvector.

Note that the eigenvalues of a real-valued matrix may generally be complex. However, (as an important special case) if the matrix \mathbf{A} is *real* and *symmetric*, *all* its eigenvalues are guaranteed to be *real*.

Example

For the real-valued (non-symmetric) 2×2 matrix

$$\mathbf{A} = \begin{pmatrix} 3 & -2 \\ -4 & 1 \end{pmatrix},$$

the two eigenvalues and their associated eigenvectors are

$$\lambda_1 = 5, \quad \mathbf{x}_1 = s \cdot \begin{pmatrix} 4 \\ -4 \end{pmatrix}, \quad \text{and} \quad \lambda_2 = -1, \quad \mathbf{x}_2 = s \cdot \begin{pmatrix} -2 \\ -4 \end{pmatrix},$$

for any nonzero $s \in \mathbb{R}$. The result can be easily verified by inserting pairs $\langle \lambda_1, \mathbf{x}_1 \rangle$ and $\langle \lambda_2, \mathbf{x}_2 \rangle$, respectively, into Eqn. (B.24).

B.4.1 Calculation of Eigenvalues

Special case: 2×2 matrix

For the special (but frequent) case of $n = 2$, the solution can be found in closed form (and without any software libraries). In this case, the characteristic equation (Eqn. (B.26)) reduces to

```

1: RealEigenValues2x2 ( $A, B, C, D$ )
   Input:  $A, B, C, D \in \mathbb{R}$ , the elements of a real-valued  $2 \times 2$  matrix  $\mathbf{A} = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$ . Returns an ordered sequence of real-valued eigenpairs  $\langle \lambda_i, \mathbf{x}_i \rangle$  for  $\mathbf{A}$ , or nil if the matrix has no real-valued eigenvalues.
2:  $R \leftarrow \frac{A+D}{2}$ 
3:  $S \leftarrow \frac{A-D}{2}$ 
4: if  $(S^2 + B \cdot C) < 0$  then
5:   return nil ▷  $\mathbf{A}$  has no real-valued eigenvalues
6: else
7:    $T \leftarrow \sqrt{S^2 + B \cdot C}$ 
8:    $\lambda_1 \leftarrow R + T$  ▷ eigenvalue  $\lambda_1$ 
9:    $\lambda_2 \leftarrow R - T$  ▷ eigenvalue  $\lambda_2$ 
10:  if  $(A - D) \geq 0$  then
11:     $\mathbf{x}_1 \leftarrow (S + T, C)^\top$  ▷ eigenvector  $\mathbf{x}_1$ 
12:     $\mathbf{x}_2 \leftarrow (B, -S - T)^\top$  ▷ eigenvector  $\mathbf{x}_2$ 
13:  else
14:     $\mathbf{x}_1 \leftarrow (B, -S + T)^\top$  ▷ eigenvector  $\mathbf{x}_1$ 
15:     $\mathbf{x}_2 \leftarrow (S - T, C)^\top$  ▷ eigenvector  $\mathbf{x}_2$ 
16:  return  $(\langle \lambda_1, \mathbf{x}_1 \rangle, \langle \lambda_2, \mathbf{x}_2 \rangle)$  ▷  $\lambda_1 \geq \lambda_2$ 

```

Alg. B.1
Calculating the real eigenvalues and eigenvectors for a 2×2 real-valued matrix \mathbf{A} . If the matrix has real eigenvalues, an ordered sequence of two “eigenpairs” $\langle \lambda_i, \mathbf{x}_i \rangle$, each containing the eigenvalue λ_i and the associated eigenvector \mathbf{x}_i , is returned ($i = 1, 2$). The resulting sequence is ordered by decreasing eigenvalues. nil is returned if \mathbf{A} has no real eigenvalues.

$$\det(\mathbf{A} - \lambda \cdot \mathbf{I}_2) = \left| \begin{pmatrix} A & B \\ C & D \end{pmatrix} - \lambda \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right| = \begin{vmatrix} A-\lambda & B \\ C & D-\lambda \end{vmatrix} \quad (\text{B.28})$$

$$= \lambda^2 - (A + D) \cdot \lambda + (AD - BC) = 0. \quad (\text{B.29})$$

The two possible solutions to this quadratic equation,

$$\begin{aligned} \lambda_{1,2} &= \frac{A + D}{2} \pm \left[\left(\frac{A + D}{2} \right)^2 - (AD - BC) \right]^{1/2} \\ &= \frac{A + D}{2} \pm \left[\left(\frac{A - D}{2} \right)^2 + BC \right]^{1/2} \\ &= R \pm \sqrt{S^2 + BC}, \end{aligned} \quad (\text{B.30})$$

are the eigenvalues of the matrix \mathbf{A} , with

$$\begin{aligned} \lambda_1 &= R + \sqrt{S^2 + B \cdot C}, \\ \lambda_2 &= R - \sqrt{S^2 + B \cdot C}. \end{aligned} \quad (\text{B.31})$$

Both λ_1, λ_2 are real-valued if the term under the square root is positive, that is, if

$$S^2 + B \cdot C = \left(\frac{A - D}{2} \right)^2 + B \cdot C \geq 0. \quad (\text{B.32})$$

In particular, if the matrix is *symmetric* (i.e., $B = C$), this condition is guaranteed (because $B \cdot C \geq 0$). In this case, $\lambda_1 \geq \lambda_2$. Algorithm B.1⁴ summarizes the closed-form computation of the eigenvalues and eigenvectors of a 2×2 matrix.

⁴ See [27] and its reprint in [28, Ch. 5].

General case: $n \times n$

In general, proven numerical software should be used for eigenvalue calculations. See the example using the Apache Commons Math library in Sec. B.6.5.

B.5 Homogeneous Coordinates

Homogeneous coordinates are an alternative representation of points in multi-dimensional space. They are commonly used in 2D and 3D geometry because they can greatly simplify the description of certain transformations. For example, affine and projective transformations become matrices with homogeneous coordinates and the composition of transformations can be performed by simple matrix multiplication.⁵

To convert a given n -dimensional *Cartesian* point $\mathbf{x} = (x_0, \dots, x_{n-1})^\top$ to *homogeneous* coordinates $\underline{\mathbf{x}}$, we use the notation⁶

$$\text{hom}(\mathbf{x}) = \underline{\mathbf{x}}. \quad (\text{B.33})$$

This operation increases the dimensionality of the original vector by one by inserting the additional element 1, that is,

$$\text{hom} \begin{pmatrix} x_0 \\ \vdots \\ x_{n-1} \end{pmatrix} = \begin{pmatrix} x_0 \\ \vdots \\ x_{n-1} \\ 1 \end{pmatrix} = \begin{pmatrix} \underline{x}_0 \\ \vdots \\ \underline{x}_{n-1} \\ \underline{x}_n \end{pmatrix}. \quad (\text{B.34})$$

Note that the homogeneous representation of a Cartesian vector is not unique, but every multiple of the homogeneous vector is an equivalent representation of \mathbf{x} . Thus any scaled homogeneous vector $\underline{\mathbf{x}}' = s \cdot \underline{\mathbf{x}}$ (with $s \in \mathbb{R}$, $s \neq 0$) corresponds to the *same* Cartesian vector (see also Eqn. (B.39)).

To convert a given homogeneous point $\underline{\mathbf{x}} = (\underline{x}_0, \dots, \underline{x}_n)^\top$ back to Cartesian coordinates \mathbf{x} we simply write

$$\text{hom}^{-1}(\underline{\mathbf{x}}) = \mathbf{x}. \quad (\text{B.35})$$

This operation can be easily derived as

$$\text{hom}^{-1} \begin{pmatrix} \underline{x}_0 \\ \vdots \\ \underline{x}_{n-1} \\ \underline{x}_n \end{pmatrix} = \frac{1}{\underline{x}_n} \cdot \begin{pmatrix} \underline{x}_0 \\ \vdots \\ \underline{x}_{n-1} \end{pmatrix} = \begin{pmatrix} x_0 \\ \vdots \\ x_{n-1} \end{pmatrix}, \quad (\text{B.36})$$

provided that $\underline{x}_n \neq 0$. Two homogeneous points $\underline{\mathbf{x}}_1$, $\underline{\mathbf{x}}_2$ are considered *equivalent* (\equiv), if they represent the same Cartesian point, that is,

$$\underline{\mathbf{x}}_1 \equiv \underline{\mathbf{x}}_2 \Leftrightarrow \text{hom}^{-1}(\underline{\mathbf{x}}_1) = \text{hom}^{-1}(\underline{\mathbf{x}}_2). \quad (\text{B.37})$$

It follows from Eqn. (B.36) that

⁵ See Chapter 21, Sec. 21.1.2.

⁶ The operator $\text{hom}()$ is introduced here for convenience and clarity.

$$\text{hom}^{-1}(\underline{\boldsymbol{x}}) = \text{hom}^{-1}(s \cdot \underline{\boldsymbol{x}}) \quad (\text{B.38})$$

for any nonzero factor $s \in \mathbb{R}$. Thus, as mentioned earlier, any scaled homogeneous point corresponds to the same Cartesian point, that is,

$$\underline{\boldsymbol{x}} \equiv s \cdot \underline{\boldsymbol{x}}. \quad (\text{B.39})$$

For example, for the Cartesian point $\boldsymbol{x} = (3, 7, 2)^\top$, the homogeneous coordinates

$$\text{hom}(\boldsymbol{x}) = \begin{pmatrix} 3 \\ 7 \\ 2 \\ 1 \end{pmatrix} \equiv \begin{pmatrix} -3 \\ -7 \\ -2 \\ -1 \end{pmatrix} \equiv \begin{pmatrix} 9 \\ 31 \\ 6 \\ 3 \end{pmatrix} \equiv \begin{pmatrix} 30 \\ 70 \\ 20 \\ 10 \end{pmatrix} \dots \quad (\text{B.40})$$

are all equivalent. Homogeneous coordinates can be used for vector spaces of arbitrary dimension, including 2D coordinates.

B.6 Basic Matrix-Vector Operations with the *Apache Commons Math* Library

It is recommended to use proven standard software, such as the *Apache Commons Math*⁷ (ACM) library, for any non-trivial linear algebra calculation.

B.6.1 Vectors and Matrices

The basic data structures for representing vectors and matrices are `RealVector` and `RealMatrix`, respectively. The following ACM examples show the conversion from and to simple Java arrays of element-type `double`:

```
import org.apache.commons.math3.linear.MatrixUtils;
import org.apache.commons.math3.linear.RealMatrix;
import org.apache.commons.math3.linear.RealVector;

// Data given as simple arrays:
double[] xa = {1, 2, 3};
double[][] Aa = {{2, 0, 1}, {0, 2, 0}, {1, 0, 2}};

// Conversion to vectors and matrices:
RealVector x = MatrixUtils.createRealVector(xa);
RealMatrix A = MatrixUtils.createRealMatrix(Aa);

// Get a single matrix element  $A_{i,j}$ :
int i, j; // specify row (i) and column (j)
double aij = A.getEntry(i, j);

// Set a single matrix element to a new value:
double value;
A.setEntry(i, j, value);

// Extract data to arrays again:
double[] xb = x.toArray();
double[][] Ab = A.getData();
```

⁷ <http://commons.apache.org/math/>.

```
// Transpose the matrix A:  
RealMatrix At = A.transpose();
```

B.6.2 Matrix-Vector Multiplication

The following examples show how to implement the various matrix-vector products described in Sec. B.2.3.

```
RealMatrix A = ...; // matrix A of size (m, n)  
RealMatrix B = ...; // matrix B of size (p, q), with p = n  
RealVector x = ...; // vector x of length n  
  
// Scalar multiplication  $C \leftarrow s \cdot A$ :  
double s = ...;  
RealMatrix C = A.scalarMultiply(s);  
  
// Product of two matrices:  $C \leftarrow A \cdot B$ :  
RealMatrix C = A.multiply(B); // C is of size (m, q)  
  
// Left-sided matrix-vector product:  $y \leftarrow A \cdot x$ :  
RealVector y = A.operate(x);  
  
// Right-sided matrix-vector product:  $y \leftarrow x^T \cdot A$ :  
RealVector y = A.preMultiply(x);
```

B.6.3 Vector Products

The following code segments show the use of the ACM library for calculating various vector products described in Sec. B.3.

```
RealVector a, b; // vectors a, b (both of length n)  
  
// Multiplication by a scalar  $c \leftarrow s \cdot a$ :  
double s;  
RealVector c = a.mapMultiply(s);  
  
// Dot (scalar) product  $x \leftarrow a \cdot b$ :  
double x = a.dotProduct(b);  
  
// Outer product  $M \leftarrow a \otimes b$ :  
RealMatrix M = a.outerProduct(b);
```

B.6.4 Inverse of a Square Matrix

The following example shows the inversion of a square matrix:

```
RealMatrix A = ...; // a square matrix  
RealMatrix Ai = MatrixUtils.inverse(A);
```

B.6.5 Eigenvalues and Eigenvectors

The following code segment illustrates the calculation of eigenvalues and eigenvectors of a square matrix A using the class `EigenDecomposition` of the Apache Commons Math API. Note that the eigenval-

ues returned by `getRealEigenvalues()` are sorted in non-increasing order. The same ordering applies to the associated eigenvectors.

```
import org.apache.commons.math3.linear.EigenDecomposition;
...

RealMatrix A = MatrixUtils.createRealMatrix(new double[] []
    {{2, 0, 1},
     {0, 2, 0},
     {1, 0, 2}});

EigenDecomposition ed = new EigenDecomposition(A);

if (ed.hasComplexEigenvalues()) {
    System.out.println("A has complex Eigenvalues!");
}
else {
    // get all real eigenvalues:
    double[] lambda = ed.getRealEigenvalues(); // = (3, 2, 1)
    // get the associated eigenvectors:
    for (int i = 0; i < lambda.length; i++) {
        RealVector x = ed.getEigenvector(i);
        ...
    }
}
```

B.7 Solving Systems of Linear Equations

This section describes standard methods for solving systems of linear equations. Such systems appear widely and frequently in all sorts of engineering problems. Identifying them and knowing about standard solution methods is thus quite important and may save much time in any development process. In addition, the solution techniques presented here are very mature and numerically stable. Note that this section is supposed to give only a brief summary of the topic and practical implementations using the Apache Commons Math library. Further details and the underlying theory can be found in most linear algebra textbooks (e.g., [145, 190]).

Systems of linear equations generally come in the form

$$\begin{pmatrix} A_{0,0} & A_{0,1} & \cdots & A_{0,n-1} \\ A_{1,0} & A_{1,1} & \cdots & A_{1,n-1} \\ A_{2,0} & A_{2,1} & \cdots & A_{2,n-1} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m-1,0} & A_{m-1,1} & \cdots & A_{m-1,n-1} \end{pmatrix} \cdot \begin{pmatrix} x_0 \\ x_1 \\ \vdots \\ x_{n-1} \end{pmatrix} = \begin{pmatrix} b_0 \\ b_1 \\ b_2 \\ \vdots \\ b_{m-1} \end{pmatrix}, \quad (\text{B.41})$$

or, in the standard notation,

$$\mathbf{A} \cdot \mathbf{x} = \mathbf{b}, \quad (\text{B.42})$$

where the (known) matrix \mathbf{A} is of size (m, n) , the *unknown* vector \mathbf{x} is n -dimensional, and the (known) vector \mathbf{b} is m -dimensional. Thus n corresponds to the number of unknowns and m to the number

of equations. Each row i of the matrix \mathbf{A} thus represents a single equation

$$A_{i,0} \cdot x_0 + A_{i,1} \cdot x_1 + \dots + A_{i,n-1} \cdot x_{n-1} = b_i \quad (\text{B.43})$$

$$\text{or} \quad \sum_{j=0}^{n-1} A_{i,j} \cdot x_j = b_i, \quad (\text{B.44})$$

for $i = 0, \dots, m-1$. Depending on m and n , the following situations may occur:

- If $m = n$ (i.e., \mathbf{A} is square) the number of unknowns matches the number of equations and the system typically (but not always, of course) has a unique solution (see Sec. B.7.1 below).
- If $m < n$, we have more unknowns than equations. In this case no unique solution exists (but possibly infinitely many).
- With $m > n$ the system is said to be *over-determined* and thus not solvable in general. Nevertheless, this is a frequent case that is typically handled by calculating a minimum least squares solution (see Sec. B.7.2).

B.7.1 Exact Solutions

If the number of equations (m) is equal to the number of unknowns (n) and the resulting (square) matrix \mathbf{A} is non-singular and of full rank $m = n$, the system $\mathbf{A} \cdot \mathbf{x} = \mathbf{b}$ can be expected to have a unique solution for \mathbf{x} . For example, the system⁸

$$\begin{aligned} 2 \cdot x_0 + 3 \cdot x_1 - 2 \cdot x_2 &= 1, \\ -x_0 + 7 \cdot x_1 + 6 \cdot x_2 &= -2, \\ 4 \cdot x_0 - 3 \cdot x_1 - 5 \cdot x_2 &= 1, \end{aligned} \quad (\text{B.45})$$

with

$$\mathbf{A} = \begin{pmatrix} 2 & 3 & -2 \\ -1 & 7 & 6 \\ 4 & -3 & -5 \end{pmatrix}, \quad \mathbf{x} = \begin{pmatrix} x_0 \\ x_1 \\ x_2 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix}, \quad (\text{B.46})$$

has the unique solution $\mathbf{x} = (-0.3698, 0.1780, -0.6027)^\top$. The following code segment shows how the previous example is solved using class `LUdecomposition` of the ACM library:

```
import org.apache...linear.DecompositionSolver;
import org.apache...linear.LUdecomposition;

RealMatrix A = MatrixUtils.createRealMatrix(new double[][]
    {{ 2, 3, -2},
     {-1, 7, 6},
     { 4, -3, -5}});
RealVector b = MatrixUtils.createRealVector(new double[]
    {1, -2, 1});
DecompositionSolver solver =
    new LUdecomposition(A).getSolver();
RealVector x = solver.solve(b);
```

An exception is thrown if the matrix \mathbf{A} is non-square or singular.

⁸ Example taken from the *Apache Commons Math User Guide* [4].

B.7.2 Over-Determined System (Least-Squares Solutions)

If a system of linear equations has more equations than unknowns (i.e., $m > n$) it is over-determined and thus has no exact solution. In other words, there is no vector \mathbf{x} that satisfies $\mathbf{A} \cdot \mathbf{x} = \mathbf{b}$ or

$$\mathbf{A} \cdot \mathbf{x} - \mathbf{b} = \mathbf{0}. \quad (\text{B.47})$$

Instead, *any* \mathbf{x} plugged into Eqn. (B.47) yields some non-zero “residual” vector $\boldsymbol{\epsilon}$, such that

$$\mathbf{A} \cdot \mathbf{x} - \mathbf{b} = \boldsymbol{\epsilon}. \quad (\text{B.48})$$

A “best” solution is commonly found by minimizing the squared norm of this residual, that is, by searching for \mathbf{x} such that

$$\|\mathbf{A} \cdot \mathbf{x} - \mathbf{b}\|^2 = \|\boldsymbol{\epsilon}\|^2 \rightarrow \min. \quad (\text{B.49})$$

Several matrix decompositions can be used for calculating the “least-squares solution” of an over-determined system of linear equations. As a simple example, we add a fourth line ($m = 4$) to the system in Eqns. (B.45) and (B.46) to

$$\mathbf{A} = \begin{pmatrix} 2 & 3 & -2 \\ -1 & 7 & 6 \\ 4 & -3 & -5 \\ 2 & -2 & -1 \end{pmatrix}, \quad \mathbf{x} = \begin{pmatrix} x_0 \\ x_1 \\ x_2 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 1 \\ -2 \\ 1 \\ 0 \end{pmatrix}, \quad (\text{B.50})$$

without changing the number of unknowns ($n = 3$). The least-squares solution to this over-determined system is (approx.) $\mathbf{x} = (-0.2339, 0.1157, -0.4942)^\top$. The following code segment shows the calculation using the `SingularValueDecomposition` class of the ACM library:

```
import org.apache...linear.DecompositionSolver;
import org.apache...linear.SingularValueDecomposition;

RealMatrix A = MatrixUtils.createRealMatrix(new double[][] {
    {2, 3, -2},
    {-1, 7, 6},
    {4, -3, -5},
    {2, -2, -1}});
RealVector b = MatrixUtils.createRealVector(new double[] {
    1, -2, 1, 0});
DecompositionSolver solver =
    new SingularValueDecomposition(A).getSolver();
RealVector x = solver.solve(b);
```

Alternatively, an instance of `QRDecomposition` could be used for calculating the least-squares solution. If an *exact* solution exists (see Sec. B.7.1), it is the same as the least-squares solution (with zero residual $\boldsymbol{\epsilon} = \mathbf{0}$).

Appendix C

Calculus

This part outlines selected topics from calculus that may serve as a useful supplement to Chapters 6, 16, 17, 24, and 25, in particular.

C.1 Parabolic Fitting

Given a single-variable (1D), discrete function $g: \mathbb{Z} \mapsto \mathbb{R}$, it is sometimes useful to locally fit a quadratic (parabolic) function, for example, for precisely locating a maximum or minimum position.

C.1.1 Fitting a Parabolic Function to Three Sample Points

For a quadratic function (second-order polynomial)

$$y = f(x) = a \cdot x^2 + b \cdot x + c \quad (\text{C.1})$$

with parameters a, b, c to pass through a given set of three sample points $\mathbf{p}_i = (x_i, y_i)$, $i = 1, 2, 3$, means that the following three equations must be satisfied:

$$\begin{aligned} y_1 &= a \cdot x_1^2 + b \cdot x_1 + c, \\ y_2 &= a \cdot x_2^2 + b \cdot x_2 + c, \\ y_3 &= a \cdot x_3^2 + b \cdot x_3 + c. \end{aligned} \quad (\text{C.2})$$

Written in the standard matrix form $\mathbf{A} \cdot \mathbf{x} = \mathbf{b}$, or

$$\begin{pmatrix} x_1^2 & x_1 & 1 \\ x_2^2 & x_2 & 1 \\ x_3^2 & x_3 & 1 \end{pmatrix} \cdot \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}, \quad (\text{C.3})$$

the unknown coefficient vector $\mathbf{x} = (a, b, c)^\top$ is directly found as

$$\mathbf{x} = \mathbf{A}^{-1} \cdot \mathbf{b} = \begin{pmatrix} x_1^2 & x_1 & 1 \\ x_2^2 & x_2 & 1 \\ x_3^2 & x_3 & 1 \end{pmatrix}^{-1} \cdot \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}, \quad (\text{C.4})$$

assuming that the matrix \mathbf{A} has a non-zero determinant. Geometrically this means that the points \mathbf{p}_i must not be *collinear*.

Example:

Fitting the sample points $\mathbf{p}_1 = (-2, 5)^\top$, $\mathbf{p}_2 = (-1, 6)^\top$, $\mathbf{p}_3 = (3, -10)^\top$ to a quadratic function, the equation to solve is (analogous to Eqn. (C.3))

$$\begin{pmatrix} 4 & -2 & 1 \\ 1 & -1 & 1 \\ 9 & 3 & 1 \end{pmatrix} \cdot \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} 5 \\ 6 \\ -10 \end{pmatrix}, \tag{C.5}$$

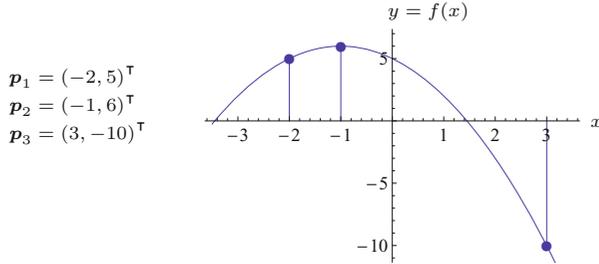
with the solution

$$\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} 4 & -2 & 1 \\ 1 & -1 & 1 \\ 9 & 3 & 1 \end{pmatrix}^{-1} \cdot \begin{pmatrix} 5 \\ 6 \\ -10 \end{pmatrix} = \frac{1}{20} \cdot \begin{pmatrix} 4 & -5 & 1 \\ -8 & 5 & 3 \\ -12 & 30 & 2 \end{pmatrix} \cdot \begin{pmatrix} 5 \\ 6 \\ -10 \end{pmatrix} = \begin{pmatrix} -1 \\ -2 \\ 5 \end{pmatrix}.$$

Thus $a = -1$, $b = -2$, $c = 5$, and the equation of the quadratic fitting function is $y = -x^2 - 2x + 5$. The result for this example is shown graphically in Fig. C.1.

Fig. C.1

Fitting a quadratic function to three arbitrary sample points.



C.1.2 Locating Extrema by Quadratic Interpolation

A special situation is when the given points are positioned at $x_1 = -1$, $x_2 = 0$, and $x_3 = +1$. This is useful, for example, to estimate a continuous extremum position from successive discrete function values defined on a regular lattice. Again the objective is to fit a quadratic function (as in Eqn. (C.1)) to pass through the points $\mathbf{p}_1 = (-1, y_1)^\top$, $\mathbf{p}_2 = (0, y_2)^\top$, and $\mathbf{p}_3 = (1, y_3)^\top$. In this case, the simultaneous equations in Eqn. (C.2) simplify to

$$\begin{aligned} y_1 &= a - b + c, \\ y_2 &= c, \\ y_3 &= a + b + c, \end{aligned} \tag{C.6}$$

with the solution

$$a = \frac{y_1 - 2 \cdot y_2 + y_3}{2}, \quad b = \frac{y_3 - y_1}{2}, \quad c = y_2. \tag{C.7}$$

To estimate a local extremum position, we take the first derivative of the quadratic fitting function (Eqn. (C.1)), which is the linear function $f'(x) = 2a \cdot x + b$, and find the position \check{x} of its (single) root by solving

$$2a \cdot x + b = 0. \tag{C.8}$$

With a, b taken from Eqn. (C.7), the extremal position is thus found as

$$\check{x} = \frac{-b}{2a} = \frac{y_1 - y_3}{2 \cdot (y_1 - 2y_2 + y_3)}. \quad (\text{C.9})$$

The corresponding extremal *value* can then be found by evaluating the quadratic function $f()$ at position \check{x} , that is,

$$\check{y} = f(\check{x}) = a \cdot \check{x}^2 + b \cdot \check{x} + c, \quad (\text{C.10})$$

with a, b, c as defined in Eqn. (C.7). **Figure C.2** shows an example with sample points $\mathbf{p}_1 = (-1, -2)^\top$, $\mathbf{p}_2 = (0, 7)^\top$, $\mathbf{p}_3 = (1, 6)^\top$. In this case, the interpolated maximum position is at $\check{x} = 0.4$ and the corresponding maximum value is $f(\check{x}) = 7.8$.

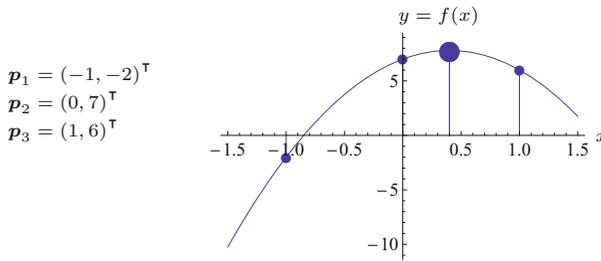


Fig. C.2

Fitting a quadratic function to three reference points at positions $x_1 = -1, x_2 = 0, x_3 = +1$. The interpolated, continuous curve has a maximum at the continuous position $\check{x} = 0.4$ (large circle).

Using the above scheme, we can interpolate any triplet of successive sample values centered around some position $u \in \mathbb{Z}$, that is, $\mathbf{p}_1 = (u - 1, y_1)^\top$, $\mathbf{p}_2 = (u, y_2)^\top$, $\mathbf{p}_3 = (u + 1, y_3)^\top$, with arbitrary values y_1, y_2, y_3 . In this case the estimated position of the extremum is simply (from Eqn. (C.9))

$$\check{x} = u + \frac{y_1 - y_3}{2 \cdot (y_1 - 2 \cdot y_2 + y_3)}. \quad (\text{C.11})$$

The application of quadratic interpolation to multi-variable functions is described in Sec. C.3.3.

C.2 Scalar and Vector Fields

An RGB color image $\mathbf{I}(u, v) = (I_R(u, v), I_G(u, v), I_B(u, v))$ can be considered a 2D function whose values are 3D vectors. Mathematically, this is a special case of a vector-valued function $\mathbf{f}: \mathbb{R}^n \mapsto \mathbb{R}^m$,

$$\mathbf{f}(\mathbf{x}) = \mathbf{f}(x_0, \dots, x_{n-1}) = \begin{pmatrix} f_0(\mathbf{x}) \\ \vdots \\ f_{m-1}(\mathbf{x}) \end{pmatrix}, \quad (\text{C.12})$$

which is composed of m scalar-valued functions $f_i: \mathbb{R}^n \mapsto \mathbb{R}$, each being defined on the domain of n -dimensional vectors.

A multi-variable, scalar-valued function $f: \mathbb{R}^n \mapsto \mathbb{R}$ is called a *scalar field*, while a vector-valued function $\mathbf{f}: \mathbb{R}^n \mapsto \mathbb{R}^m$ is referred to as a *vector field*.

C.2.1 The Jacobian Matrix

Assuming that the function $\mathbf{f}(\mathbf{x}) = (f_0(\mathbf{x}), \dots, f_{m-1}(\mathbf{x}))^\top$ is differentiable, the so-called *functional* or *Jacobian* matrix at a specific point $\dot{\mathbf{x}} = (\dot{x}_0, \dots, \dot{x}_{n-1})$ is defined as

$$\mathbf{J}_f(\dot{\mathbf{x}}) = \begin{pmatrix} \frac{\partial}{\partial x_0} f_0(\dot{\mathbf{x}}) & \cdots & \frac{\partial}{\partial x_{n-1}} f_0(\dot{\mathbf{x}}) \\ \vdots & \ddots & \vdots \\ \frac{\partial}{\partial x_0} f_{m-1}(\dot{\mathbf{x}}) & \cdots & \frac{\partial}{\partial x_{n-1}} f_{m-1}(\dot{\mathbf{x}}) \end{pmatrix}. \quad (\text{C.13})$$

The Jacobian matrix is of size $m \times n$ and composed of the first derivatives of the m component functions f_0, \dots, f_{m-1} with respect to each of the n independent variables x_0, \dots, x_{n-1} . Thus each of its elements $\frac{\partial}{\partial x_j} f_i(\dot{\mathbf{x}})$ quantifies how much the value of the scalar-valued component function $f_i(\mathbf{x}) = f_i(x_0, \dots, x_{n-1})$ changes when only variable x_j is varied and all other variables remain fixed. Note that the matrix $\mathbf{J}_f(\mathbf{x})$ is not constant for a given function \mathbf{f} but is different at each position $\dot{\mathbf{x}}$. In general, the Jacobian matrix is neither square (unless $m = n$) nor symmetric.

C.2.2 Gradients

Gradient of a scalar field

The gradient of a *scalar field* $f: \mathbb{R}^n \mapsto \mathbb{R}$, with $f(\mathbf{x}) = f(x_0, \dots, x_{n-1})$, at a given position $\dot{\mathbf{x}} \in \mathbb{R}^n$ is defined as

$$(\nabla f)(\dot{\mathbf{x}}) = (\text{grad } f)(\dot{\mathbf{x}}) = \begin{pmatrix} \frac{\partial}{\partial x_0} f(\dot{\mathbf{x}}) \\ \vdots \\ \frac{\partial}{\partial x_{n-1}} f(\dot{\mathbf{x}}) \end{pmatrix}. \quad (\text{C.14})$$

The resulting vector-valued function quantifies the amount of output change with respect to changing any of the input variables x_0, \dots, x_{n-1} at position $\dot{\mathbf{x}}$. Thus the gradient of a scalar field is a vector field.

The *directional* gradient of a scalar field describes how the (scalar) function value changes when the coordinates are modified along a particular direction, specified by the unit vector \mathbf{e} . We denote the directional gradient as $\nabla_{\mathbf{e}} f$ and define

$$(\nabla_{\mathbf{e}} f)(\dot{\mathbf{x}}) = (\nabla f)(\dot{\mathbf{x}}) \cdot \mathbf{e}, \quad (\text{C.15})$$

where \cdot is the scalar product (see Sec. B.3.1). The result is a scalar value that can be interpreted as the slope of the tangent on the n -dimensional surface of the scalar field at position $\dot{\mathbf{x}}$ along the direction specified by the n -dimensional unit vector $\mathbf{e} = (e_0, \dots, e_{n-1})^\top$.

Gradient of a vector field

To calculate the gradient of a *vector field* $\mathbf{f}: \mathbb{R}^n \mapsto \mathbb{R}^m$, we note that each row i in the $m \times n$ Jacobian matrix \mathbf{J}_f (Eqn. (C.13)) is the transposed gradient vector of the corresponding component function f_i , that is,

$$\mathbf{J}_f(\dot{\mathbf{x}}) = \begin{pmatrix} (\nabla f_0)(\dot{\mathbf{x}})^\top \\ \vdots \\ (\nabla f_{m-1})(\dot{\mathbf{x}})^\top \end{pmatrix}, \quad (\text{C.16})$$

and thus the Jacobian matrix is equivalent to the gradient of the vector field \mathbf{f} ,

$$(\text{grad } \mathbf{f})(\dot{\mathbf{x}}) \equiv \mathbf{J}_f(\dot{\mathbf{x}}). \quad (\text{C.17})$$

Analogous to Eqn. (C.15), the *directional* gradient of the vector field is then defined as

$$(\text{grad}_{\mathbf{e}} \mathbf{f})(\dot{\mathbf{x}}) \equiv \mathbf{J}_f(\dot{\mathbf{x}}) \cdot \mathbf{e}, \quad (\text{C.18})$$

where \mathbf{e} is again a unit vector specifying the gradient direction and \cdot is the ordinary matrix-vector product. In this case the resulting gradient is a m -dimensional vector with one element for each component function in \mathbf{f} .

C.2.3 Maximum Gradient Direction

In case of a scalar field $f(\mathbf{x})$, a resulting non-zero gradient vector $(\nabla f)(\dot{\mathbf{x}})$ (Eqn. (C.14)) is also the direction of the steepest ascent of $f(\mathbf{x})$ at position $\dot{\mathbf{x}}$.¹ In this case, the L_2 norm (see Sec. B.1.2) of the gradient vector, that is, $\|(\nabla f)(\dot{\mathbf{x}})\|$, corresponds to the maximum slope of f at point $\dot{\mathbf{x}}$.

In case of a vector field $\mathbf{f}(\mathbf{x})$, the direction of maximum slope cannot be obtained directly, since the gradient is not a n -dimensional vector but its $m \times n$ Jacobian matrix. In this case, the direction of maximum change in the function \mathbf{f} is found as the eigenvector \mathbf{x}_k of the square ($n \times n$) matrix

$$\mathbf{M} = \mathbf{J}_f^\top(\dot{\mathbf{x}}) \cdot \mathbf{J}_f(\dot{\mathbf{x}}) \quad (\text{C.19})$$

that corresponds to its largest eigenvalue λ_k (see also Sec. B.4).

C.2.4 Divergence of a Vector Field

If the vector field maps to the same vector space (i.e., $\mathbf{f}: \mathbb{R}^n \mapsto \mathbb{R}^n$), its *divergence* (div) is defined as

$$(\text{div } \mathbf{f})(\dot{\mathbf{x}}) = \frac{\partial}{\partial x_0} f_0(\dot{\mathbf{x}}) + \cdots + \frac{\partial}{\partial x_{n-1}} f_{n-1}(\dot{\mathbf{x}}) \quad (\text{C.20})$$

$$= \sum_{i=0}^{n-1} \frac{\partial}{\partial x_i} f_i(\dot{\mathbf{x}}) \in \mathbb{R}, \quad (\text{C.21})$$

for a given point $\dot{\mathbf{x}}$. The result is a scalar value and thus $(\text{div } \mathbf{f})(\dot{\mathbf{x}})$ yields a scalar field $\mathbb{R}^n \mapsto \mathbb{R}$. Note that, in this case, the Jacobian matrix \mathbf{J}_f in Eqn. (C.13) is square (of size $n \times n$) and $\text{div } \mathbf{f}$ is equivalent to the trace of \mathbf{J}_f , that is,

$$(\text{div } \mathbf{f})(\dot{\mathbf{x}}) \equiv \text{trace}(\mathbf{J}_f(\dot{\mathbf{x}})). \quad (\text{C.22})$$

¹ If the gradient vector is *zero*, that is, if $(\nabla f)(\dot{\mathbf{x}}) = \mathbf{0}$, the direction of the gradient is undefined at position $\dot{\mathbf{x}}$.

C.2.5 Laplacian Operator

The *Laplacian* (or Laplace operator) of a scalar field $f: \mathbb{R}^n \mapsto \mathbb{R}$ is a linear differential operator, commonly denoted Δ or ∇^2 . The result of applying ∇^2 to the scalar field $f: \mathbb{R}^n \mapsto \mathbb{R}$ generates another scalar field that consists of the sum of all unmixed second-order partial derivatives of f (if existent), that is,

$$(\nabla^2 f)(\dot{\mathbf{x}}) = \frac{\partial^2}{\partial x_0^2} f(\dot{\mathbf{x}}) + \cdots + \frac{\partial^2}{\partial x_{n-1}^2} f(\dot{\mathbf{x}}) = \sum_{i=0}^{n-1} \frac{\partial^2}{\partial x_i^2} f(\dot{\mathbf{x}}). \quad (\text{C.23})$$

The result is a scalar value that is equivalent to the *divergence* (see Eqn. (C.21)) of the *gradient* (see Eqn. (C.14)) of the scalar field f , that is,

$$(\nabla^2 f)(\dot{\mathbf{x}}) = (\text{div} \nabla f)s(\dot{\mathbf{x}}). \quad (\text{C.24})$$

The *Laplacian* is also found as the *trace* of the function's Hessian matrix \mathbf{H}_f (see Sec. C.2.6).

For a *vector-valued* function $\mathbf{f}: \mathbb{R}^n \mapsto \mathbb{R}^m$, the Laplacian at point $\dot{\mathbf{x}}$ is again a vector field $\mathbb{R}^n \mapsto \mathbb{R}^m$,

$$(\nabla^2 \mathbf{f})(\dot{\mathbf{x}}) = \begin{pmatrix} (\nabla^2 f_0)(\dot{\mathbf{x}}) \\ (\nabla^2 f_1)(\dot{\mathbf{x}}) \\ \vdots \\ (\nabla^2 f_{m-1})(\dot{\mathbf{x}}) \end{pmatrix} \in \mathbb{R}^m, \quad (\text{C.25})$$

that is obtained by applying the Laplacian to the individual (scalar-valued) component functions.

C.2.6 The Hessian Matrix

The Hessian matrix of a n -variable, real-valued function $f: \mathbb{R}^n \mapsto \mathbb{R}$ is the $n \times n$ square matrix composed of its second-order partial derivatives (assuming they all exist), that is,

$$\mathbf{H}_f = \begin{pmatrix} H_{0,0} & H_{0,1} & \cdots & H_{0,n-1} \\ H_{1,0} & H_{1,1} & \cdots & H_{1,n-1} \\ \vdots & \vdots & \ddots & \vdots \\ H_{n-1,0} & H_{n-1,1} & \cdots & H_{n-1,n-1} \end{pmatrix} \quad (\text{C.26})$$

$$= \begin{pmatrix} \frac{\partial^2}{\partial x_0^2} f & \frac{\partial^2}{\partial x_0 \partial x_1} f & \cdots & \frac{\partial^2}{\partial x_0 \partial x_{n-1}} f \\ \frac{\partial^2}{\partial x_1 \partial x_0} f & \frac{\partial^2}{\partial x_1^2} f & \cdots & \frac{\partial^2}{\partial x_1 \partial x_{n-1}} f \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2}{\partial x_{n-1} \partial x_0} f & \frac{\partial^2}{\partial x_{n-1} \partial x_1} f & \cdots & \frac{\partial^2}{\partial x_{n-1}^2} f \end{pmatrix}. \quad (\text{C.27})$$

Since the order of differentiation does not matter (i.e., $H_{i,j} = H_{j,i}$), \mathbf{H}_f is symmetric. Note that the Hessian is a matrix of *functions*. To evaluate the Hessian at a particular point $\dot{\mathbf{x}} \in \mathbb{R}^n$, we write

$$\mathbf{H}_f(\dot{\mathbf{x}}) = \begin{pmatrix} \frac{\partial^2}{\partial x_0^2} f(\dot{\mathbf{x}}) & \cdots & \frac{\partial^2}{\partial x_0 \partial x_{n-1}} f(\dot{\mathbf{x}}) \\ \vdots & \ddots & \vdots \\ \frac{\partial^2}{\partial x_{n-1} \partial x_0} f(\dot{\mathbf{x}}) & \cdots & \frac{\partial^2}{\partial x_{n-1}^2} f(\dot{\mathbf{x}}) \end{pmatrix}, \quad (\text{C.28})$$

which is a scalar-valued matrix of size $n \times n$. As mentioned already, the *trace* of the Hessian matrix is the *Laplacian* ∇^2 of the function f , that is,

$$\nabla^2 f = \text{trace}(\mathbf{H}_f) = \sum_{i=0}^{n-1} \frac{\partial^2}{\partial x_i^2} f. \quad (\text{C.29})$$

Example

Given a 2D, continuous, grayscale image or scalar-valued intensity function $I(x, y)$, the corresponding Hessian matrix (of size 2×2) contains all second derivatives along the coordinates x, y , that is,

$$\mathbf{H}_I = \begin{pmatrix} \frac{\partial^2}{\partial x^2} I & \frac{\partial^2}{\partial x \partial y} I \\ \frac{\partial^2}{\partial y \partial x} I & \frac{\partial^2}{\partial y^2} I \end{pmatrix} = \begin{pmatrix} I_{xx} & I_{xy} \\ I_{yx} & I_{yy} \end{pmatrix}, \quad (\text{C.30})$$

The elements of \mathbf{H}_I are 2D, scalar-valued functions over x, y and thus scalar fields again. Evaluating the Hessian matrix at a particular point $\dot{\mathbf{x}}$ yields the values of the second partial derivatives of I at this position,

$$\mathbf{H}_I(\dot{\mathbf{x}}) = \begin{pmatrix} \frac{\partial^2}{\partial x^2} I(\dot{\mathbf{x}}) & \frac{\partial^2}{\partial x \partial y} I(\dot{\mathbf{x}}) \\ \frac{\partial^2}{\partial y \partial x} I(\dot{\mathbf{x}}) & \frac{\partial^2}{\partial y^2} I(\dot{\mathbf{x}}) \end{pmatrix} = \begin{pmatrix} I_{xx}(\dot{\mathbf{x}}) & I_{xy}(\dot{\mathbf{x}}) \\ I_{yx}(\dot{\mathbf{x}}) & I_{yy}(\dot{\mathbf{x}}) \end{pmatrix}, \quad (\text{C.31})$$

that is, a matrix with scalar-valued elements.

C.3 Operations on Multi-Variable, Scalar Functions (Scalar Fields)

C.3.1 Estimating the Derivatives of a Discrete Function

Images are typically discrete functions (i.e., $I: \mathbb{N}^2 \mapsto \mathbb{R}$) and thus not differentiable. The derivatives can nevertheless be estimated by calculating finite differences from the pixel values in a 3×3 neighborhood, which can be expressed as a linear filter or convolution operation ($*$). In particular, the *first-order* derivatives $I_x = \partial I / \partial x$ and $I_y = \partial I / \partial y$ are usually estimated in the form

$$I_x \approx I * \begin{bmatrix} -0.5 & \mathbf{0} & 0.5 \end{bmatrix}, \quad I_y \approx I * \begin{bmatrix} -0.5 \\ \mathbf{0} \\ 0.5 \end{bmatrix}, \quad (\text{C.32})$$

the second-order derivatives $I_{xx} = \partial^2 I / \partial x^2$ and $I_{yy} = \partial^2 I / \partial y^2$ as

$$I_{xx} \approx I * \begin{bmatrix} 1 & -2 & 1 \end{bmatrix}, \quad I_{yy} \approx I * \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}, \quad (\text{C.33})$$

and the mixed derivative

$$\begin{aligned} \frac{\partial^2 I}{\partial x \partial y} &= I_{xy} = I_{yx} \\ &\approx I * [-0.5 \quad \mathbf{0} \quad 0.5] * \begin{bmatrix} -0.5 \\ \mathbf{0} \\ 0.5 \end{bmatrix} = I * \begin{bmatrix} 0.25 & 0 & -0.25 \\ 0 & \mathbf{0} & 0 \\ -0.25 & 0 & 0.25 \end{bmatrix}. \end{aligned} \quad (\text{C.34})$$

C.3.2 Taylor Series Expansion of Functions

Single-variable functions

The Taylor series expansion (of degree d) of a single-variable function $f: \mathbb{R} \mapsto \mathbb{R}$ about a reference point a is

$$\begin{aligned} f(x) &= f(a) + f'(a) \cdot (x-a) + f''(a) \cdot \frac{(x-a)^2}{2} + \dots \\ &\quad \dots + f^{(d)}(a) \cdot \frac{(x-a)^d}{d!} + R_d \end{aligned} \quad (\text{C.35})$$

$$= f(a) + \sum_{i=1}^d f^{(i)}(a) \cdot \frac{(x-a)^i}{i!} + R_d \quad (\text{C.36})$$

$$= \sum_{i=0}^d f^{(i)}(a) \cdot \frac{(x-a)^i}{i!} + R_d, \quad (\text{C.37})$$

where R_d is the residual term.² This means that if the value $f(a)$ and the first d derivatives $f'(a), f''(a), \dots, f^{(d)}(a)$ exist and are known at some position a , the value of f at *another* point x can be estimated (up to the residual R_d) only from the values at point a , without actually evaluating $f(x)$. Omitting the remainder R_d , the result is an *approximation* for $f(x)$, that is,

$$f(x) \approx \sum_{i=0}^d f^{(i)}(a) \cdot \frac{(x-a)^i}{i!}, \quad (\text{C.38})$$

whose accuracy depends upon d and the distance $x - a$.

Multi-variable functions

In general, for a real-valued function of n variables,

$$f(\mathbf{x}) = f(x_0, x_2, \dots, x_{n-1}) \in \mathbb{R},$$

the full Taylor series expansion about a reference point $\mathbf{a} = (a_0, \dots, a_{n-1})^\top$ is

$$\begin{aligned} f(x_0, \dots, x_{n-1}) &= f(\mathbf{a}) + \\ &\quad \sum_{i_0=1}^{\infty} \dots \sum_{i_{n-1}=1}^{\infty} \left[\frac{\partial^{i_0}}{\partial x_0^{i_0}} \dots \frac{\partial^{i_{n-1}}}{\partial x_{n-1}^{i_{n-1}}} \right] f(\mathbf{a}) \cdot \frac{(x_0 - a_0)^{i_0} \dots (x_{n-1} - a_{n-1})^{i_{n-1}}}{i_1! \dots i_n!} \\ &= \sum_{i_1=0}^{\infty} \dots \sum_{i_n=0}^{\infty} \left[\frac{\partial^{i_0}}{\partial x_0^{i_0}} \dots \frac{\partial^{i_{n-1}}}{\partial x_{n-1}^{i_{n-1}}} \right] f(\mathbf{a}) \cdot \frac{(x_0 - a_0)^{i_0} \dots (x_{n-1} - a_{n-1})^{i_{n-1}}}{i_0! \dots i_{n-1}!}. \end{aligned} \quad (\text{C.39})$$

² Note that $f^{(0)} = f$, $f^{(1)} = f'$, $f^{(2)} = f''$ etc., and $1! = 1$.

In Eqn. (C.39),³ the term

$$\left[\frac{\partial^{i_0}}{\partial x_0^{i_0}} \cdots \frac{\partial^{i_{n-1}}}{\partial x_{n-1}^{i_{n-1}}} \right] f(\mathbf{a}) \quad (\text{C.40})$$

is the value of the function f , after applying a sequence of n partial derivatives, at the n -dimensional position \mathbf{a} . The operator $\frac{\partial^i}{\partial x_k^i}$ denotes the i -th partial derivative on the variable x_k .

To formulate Eqn. (C.39) in a more compact fashion, we define the index vector

$$\mathbf{i} = (i_0, i_1, \dots, i_{n-1}), \quad (\text{C.41})$$

(with $i_k \in \mathbb{N}_0$ and thus $\mathbf{i} \in \mathbb{N}_0^n$), and the associated operations

$$\begin{aligned} \mathbf{i}! &= i_0! \cdot i_1! \cdots i_{n-1}!, \\ \mathbf{x}^{\mathbf{i}} &= x_0^{i_0} \cdot x_1^{i_1} \cdots x_{n-1}^{i_{n-1}}, \\ \Sigma \mathbf{i} &= i_0 + i_1 + \cdots + i_{n-1}. \end{aligned} \quad (\text{C.42})$$

As a shorthand notation for the combined partial derivative operator in Eqn. (C.40) we define

$$D^{\mathbf{i}} := \frac{\partial^{i_0}}{\partial x_0^{i_0}} \frac{\partial^{i_1}}{\partial x_1^{i_1}} \cdots \frac{\partial^{i_{n-1}}}{\partial x_{n-1}^{i_{n-1}}} = \frac{\partial^{i_0+i_1+\dots+i_{n-1}}}{\partial x_0^{i_0} \partial x_1^{i_1} \cdots \partial x_{n-1}^{i_{n-1}}}. \quad (\text{C.43})$$

With these definitions, the full Taylor expansion of a multi-variable function about a point \mathbf{a} , as given in Eqn. (C.39), can be elegantly written in the form

$$f(\mathbf{x}) = \sum_{\mathbf{i} \in \mathbb{N}_0^n} D^{\mathbf{i}} f(\mathbf{a}) \cdot \frac{(\mathbf{x} - \mathbf{a})^{\mathbf{i}}}{\mathbf{i}!}. \quad (\text{C.44})$$

Note that $D^{\mathbf{i}} f$ is again a n -dimensional function $\mathbb{R}^n \mapsto \mathbb{R}$, and thus $[D^{\mathbf{i}} f](\mathbf{a})$ in Eqn. (C.44) is the scalar quantity obtained by evaluating the function $[D^{\mathbf{i}} f]$ at the n -dimensional point \mathbf{a} .

To obtain a Taylor *approximation* of order d , the sum of the indices i_1, \dots, i_n is limited to d , that is, the summation is constrained to index vectors \mathbf{i} , with $\Sigma \mathbf{i} \leq d$. The resulting formulation,

$$f(\mathbf{x}) \approx \sum_{\substack{\mathbf{i} \in \mathbb{N}_0^n \\ \Sigma \mathbf{i} \leq d}} D^{\mathbf{i}} f(\mathbf{a}) \cdot \frac{(\mathbf{x} - \mathbf{a})^{\mathbf{i}}}{\mathbf{i}!}, \quad (\text{C.45})$$

is obviously analogous to the 1D case in Eqn. (C.38).

Example: two-variable (2D) function

This example demonstrates the second-order ($d = 2$) Taylor expansion of a 2D ($n = 2$) function $f: \mathbb{R}^2 \mapsto \mathbb{R}$ around a point $\mathbf{a} = (x_a, y_a)$. By inserting into Eqn. (C.44), we get

³ Note that symbols x_0, \dots, x_{n-1} denote the individual variables, while $\dot{x}_0, \dots, \dot{x}_{n-1}$ are the coordinates of a specific point in n -dimensional space.

$$f(x, y) \approx \sum_{\substack{\mathbf{i} \in \mathbb{N}_0^2 \\ \Sigma \mathbf{i} \leq 2}} D^{\mathbf{i}} f(x_a, y_a) \cdot \frac{1}{\mathbf{i}!} \cdot \begin{pmatrix} x-x_a \\ y-y_a \end{pmatrix}^{\mathbf{i}} \quad (\text{C.46})$$

$$= \sum_{\substack{0 \leq i, j \leq 2 \\ (i+j) \leq 2}} \frac{\partial^{i+j}}{\partial x^i \partial y^j} f(x_a, y_a) \cdot \frac{(x-x_a)^i \cdot (y-y_a)^j}{i! \cdot j!}. \quad (\text{C.47})$$

Since $d = 2$, the six permissible index vectors $\mathbf{i} = (i, j)$, with $\Sigma \mathbf{i} \leq 2$, are $(0, 0)$, $(1, 0)$, $(0, 1)$, $(1, 1)$, $(2, 0)$, and $(0, 2)$. Inserting into Eqn. (C.47), we obtain the corresponding Taylor approximation at position (\dot{x}, \dot{y}) as

$$\begin{aligned} f(x, y) &\approx \frac{\partial^0}{\partial x^0 \partial y^0} f(x_a, y_a) \cdot \frac{(x-x_a)^0 \cdot (y-y_a)^0}{1 \cdot 1} \\ &+ \frac{\partial^1}{\partial x^1 \partial y^0} f(x_a, y_a) \cdot \frac{(x-x_a)^1 \cdot (y-y_a)^0}{1 \cdot 1} \\ &+ \frac{\partial^1}{\partial x^0 \partial y^1} f(x_a, y_a) \cdot \frac{(x-x_a)^0 \cdot (y-y_a)^1}{1 \cdot 1} \\ &+ \frac{\partial^2}{\partial x^1 \partial y^1} f(x_a, y_a) \cdot \frac{(x-x_a)^1 \cdot (y-y_a)^1}{1 \cdot 1} \\ &+ \frac{\partial^2}{\partial x^2 \partial y^0} f(x_a, y_a) \cdot \frac{(x-x_a)^2 \cdot (y-y_a)^0}{2 \cdot 1} \\ &+ \frac{\partial^2}{\partial x^0 \partial y^2} f(x_a, y_a) \cdot \frac{(x-x_a)^0 \cdot (y-y_a)^2}{1 \cdot 2} \\ &= f(x_a, y_a) \end{aligned} \quad (\text{C.48})$$

$$\begin{aligned} &+ \frac{\partial}{\partial x} f(x_a, y_a) \cdot (x-x_a) + \frac{\partial}{\partial y} f(x_a, y_a) \cdot (y-y_a) \\ &+ \frac{\partial^2}{\partial x \partial y} f(x_a, y_a) \cdot (x-x_a) \cdot (y-y_a) \\ &+ \frac{1}{2} \cdot \frac{\partial^2}{\partial x^2} f(x_a, y_a) \cdot (x-x_a)^2 + \frac{1}{2} \cdot \frac{\partial^2}{\partial y^2} f(x_a, y_a) \cdot (y-y_a)^2. \end{aligned} \quad (\text{C.49})$$

It is assumed that the required derivatives of f exist, that is, f is differentiable at point (x_a, y_a) with respect to x and y up to the second order. By slightly rearranging Eqn. (C.49) to

$$\begin{aligned} f(x, y) &\approx f(x_a, y_a) + \frac{\partial}{\partial x} f(x_a, y_a) \cdot (x-x_a) + \frac{\partial}{\partial y} f(x_a, y_a) \cdot (y-y_a) \\ &+ \frac{1}{2} \cdot \left[\frac{\partial^2}{\partial x^2} f(x_a, y_a) \cdot (x-x_a)^2 + 2 \cdot \frac{\partial^2}{\partial x \partial y} f(x_a, y_a) \cdot (x-x_a) \cdot (y-y_a) \right. \\ &\quad \left. + \frac{\partial^2}{\partial y^2} f(x_a, y_a) \cdot (y-y_a)^2 \right] \end{aligned} \quad (\text{C.50})$$

we can now write the Taylor expansion in matrix-vector notation as

$$\begin{aligned} f(x, y) &\approx \tilde{f}(x, y) = f(x_a, y_a) + \begin{pmatrix} \frac{\partial}{\partial x} f(x_a, y_a), \frac{\partial}{\partial y} f(x_a, y_a) \end{pmatrix} \cdot \begin{pmatrix} x-x_a \\ y-y_a \end{pmatrix} \\ &+ \frac{1}{2} \cdot \left[(x-x_a, y-y_a) \cdot \begin{pmatrix} \frac{\partial^2}{\partial x^2} f(x_a, y_a) & \frac{\partial^2}{\partial x \partial y} f(x_a, y_a) \\ \frac{\partial^2}{\partial x \partial y} f(x_a, y_a) & \frac{\partial^2}{\partial y^2} f(x_a, y_a) \end{pmatrix} \cdot \begin{pmatrix} x-x_a \\ y-y_a \end{pmatrix} \right] \end{aligned} \quad (\text{C.51})$$

or, even more compactly, in the form

$$\tilde{f}(\mathbf{x}) = f(\mathbf{a}) + \nabla_f^T(\mathbf{a}) \cdot (\mathbf{x}-\mathbf{a}) + \frac{1}{2} \cdot (\mathbf{x}-\mathbf{a})^T \cdot \mathbf{H}_f(\mathbf{a}) \cdot (\mathbf{x}-\mathbf{a}). \quad (\text{C.52})$$

Here $\nabla_f^\top(\mathbf{a})$ denotes the (transposed) *gradient* vector of the function f at point \mathbf{a} (see Sec. C.2.2), and \mathbf{H}_f is the 2×2 *Hessian* matrix of f (see Sec. C.2.6),

$$\mathbf{H}_f(\mathbf{a}) = \begin{pmatrix} H_{00} & H_{01} \\ H_{10} & H_{11} \end{pmatrix} = \begin{pmatrix} \frac{\partial^2}{\partial x^2} f(\mathbf{a}) & \frac{\partial^2}{\partial x \partial y} f(\mathbf{a}) \\ \frac{\partial^2}{\partial x \partial y} f(\mathbf{a}) & \frac{\partial^2}{\partial y^2} f(\mathbf{a}) \end{pmatrix}. \quad (\text{C.53})$$

If the function f is *discrete*, for example, a scalar-valued image I , the required partial derivatives at some lattice point $\mathbf{a} = (u_a, v_a)^\top$ can be estimated from its 3×3 neighborhood, as described in Sec. C.3.1.

Example: three-variable (3D) function

For a 3D function $f: \mathbb{R}^3 \mapsto \mathbb{R}$, the second-order Taylor expansion ($d = 2$) is analogous to Eqns. (C.51–C.52) for the 2D case, except that now the positions $\mathbf{x} = (x, y, z)^\top$ and $\mathbf{a} = (x_a, y_a, z_a)^\top$ are 3D vectors. The associated (transposed) gradient vector is

$$\nabla_f^\top(\mathbf{a}) = \left(\frac{\partial}{\partial x} f(\mathbf{a}), \frac{\partial}{\partial y} f(\mathbf{a}), \frac{\partial}{\partial z} f(\mathbf{a}) \right), \quad (\text{C.54})$$

and the Hessian, composed of all second-order partial derivatives, is the 3×3 matrix

$$\mathbf{H}_f(\mathbf{a}) = \begin{pmatrix} \frac{\partial^2}{\partial x^2} f(\mathbf{a}) & \frac{\partial^2}{\partial x \partial y} f(\mathbf{a}) & \frac{\partial^2}{\partial x \partial z} f(\mathbf{a}) \\ \frac{\partial^2}{\partial y \partial x} f(\mathbf{a}) & \frac{\partial^2}{\partial y^2} f(\mathbf{a}) & \frac{\partial^2}{\partial y \partial z} f(\mathbf{a}) \\ \frac{\partial^2}{\partial z \partial x} f(\mathbf{a}) & \frac{\partial^2}{\partial z \partial y} f(\mathbf{a}) & \frac{\partial^2}{\partial z^2} f(\mathbf{a}) \end{pmatrix}. \quad (\text{C.55})$$

Note that the order of differentiation is not relevant since, for example, $\frac{\partial^2}{\partial x \partial y} = \frac{\partial^2}{\partial y \partial x}$, and therefore \mathbf{H}_f is always symmetric.

This can be easily generalized to the n -dimensional case, though things become considerably more involved for Taylor expansions of higher orders ($d > 2$).

C.3.3 Finding the Continuous Extremum of a Multi-Variable Discrete Function

In Sec. C.1.2 we described how the position of a local extremum can be determined by fitting a quadratic function to the neighboring samples of a $1D$ function. This section shows how this technique can be extended to n -dimensional, scalar-valued functions $f: \mathbb{R}^n \mapsto \mathbb{R}$.

Without loss of generality we can assume that the Taylor expansion of the function $f(\mathbf{x})$ is carried out around the point $\mathbf{a} = \mathbf{0} = (0, \dots, 0)$, which clearly simplifies the remaining formulation. The Taylor approximation function (see Eqn. (C.52)) for this point can be written as

$$\tilde{f}(\mathbf{x}) = f(\mathbf{0}) + \nabla_f^\top(\mathbf{0}) \cdot \mathbf{x} + \frac{1}{2} \cdot \mathbf{x}^\top \cdot \mathbf{H}_f(\mathbf{0}) \cdot \mathbf{x}, \quad (\text{C.56})$$

with the gradient ∇_f and the Hessian matrix \mathbf{H}_f evaluated at position $\mathbf{0}$. The vector of the first derivative of this function is

$$\tilde{f}'(\mathbf{x}) = \nabla_f(\mathbf{0}) + \frac{1}{2} \cdot [(\mathbf{x}^\top \cdot \mathbf{H}_f(\mathbf{0}))^\top + \mathbf{H}_f(\mathbf{0}) \cdot \mathbf{x}]. \quad (\text{C.57})$$

Since $(\mathbf{x}^\top \cdot \mathbf{H}_f)^\top = (\mathbf{H}_f^\top \cdot \mathbf{x})$ and because the Hessian matrix \mathbf{H}_f is symmetric (i.e., $\mathbf{H}_f = \mathbf{H}_f^\top$), this simplifies to

$$\tilde{f}'(\mathbf{x}) = \nabla_f(\mathbf{0}) + \frac{1}{2} \cdot (\mathbf{H}_f(\mathbf{0}) \cdot \mathbf{x} + \mathbf{H}_f(\mathbf{0}) \cdot \mathbf{x}) \quad (\text{C.58})$$

$$= \nabla_f(\mathbf{0}) + \mathbf{H}_f(\mathbf{0}) \cdot \mathbf{x}. \quad (\text{C.59})$$

A local maximum or minimum is found where all first derivatives \tilde{f}' are zero, so we need to solve

$$\nabla_f(\mathbf{0}) + \mathbf{H}_f(\mathbf{0}) \cdot \check{\mathbf{x}} = \mathbf{0}, \quad (\text{C.60})$$

for the unknown position $\check{\mathbf{x}}$. By multiplying both sides with \mathbf{H}_f^{-1} (assuming that the inverse of $\mathbf{H}_f(\mathbf{0})$ exists), the solution is

$$\check{\mathbf{x}} = -\mathbf{H}_f^{-1}(\mathbf{0}) \cdot \nabla_f(\mathbf{0}), \quad (\text{C.61})$$

for the specific expansion point $\mathbf{a} = \mathbf{0}$ (Eqn. (C.63)). Analogously, for an arbitrary expansion point \mathbf{a} , the extremum position is

$$\check{\mathbf{x}} = \mathbf{a} - \mathbf{H}_f^{-1}(\mathbf{a}) \cdot \nabla_f(\mathbf{a}). \quad (\text{C.62})$$

Note that the inverse Hessian matrix \mathbf{H}_f^{-1} is again symmetric.

The estimated extremal *value* of the approximation function \tilde{f} is found by replacing \mathbf{x} in Eqn. (C.56) with the extremal position $\check{\mathbf{x}}$ (calculated in Eqn. (C.61)) as

$$\begin{aligned} \tilde{f}_{\text{extrm}} &= \tilde{f}(\check{\mathbf{x}}) = f(\mathbf{0}) + \nabla_f^\top(\mathbf{0}) \cdot \check{\mathbf{x}} + \frac{1}{2} \cdot \check{\mathbf{x}}^\top \cdot \mathbf{H}_f(\mathbf{0}) \cdot \check{\mathbf{x}} \\ &= f(\mathbf{0}) + \nabla_f^\top(\mathbf{0}) \cdot \check{\mathbf{x}} + \frac{1}{2} \cdot \check{\mathbf{x}}^\top \cdot \mathbf{H}_f(\mathbf{0}) \cdot (-\mathbf{H}_f^{-1}(\mathbf{0})) \cdot \nabla_f(\mathbf{0}) \\ &= f(\mathbf{0}) + \nabla_f^\top(\mathbf{0}) \cdot \check{\mathbf{x}} - \frac{1}{2} \cdot \check{\mathbf{x}}^\top \cdot \mathbf{I} \cdot \nabla_f(\mathbf{0}) \\ &= f(\mathbf{0}) + \nabla_f^\top(\mathbf{0}) \cdot \check{\mathbf{x}} - \frac{1}{2} \cdot \nabla_f^\top(\mathbf{0}) \cdot \check{\mathbf{x}} \\ &= f(\mathbf{0}) + \frac{1}{2} \cdot \nabla_f^\top(\mathbf{0}) \cdot \check{\mathbf{x}}, \end{aligned} \quad (\text{C.63})$$

again for the expansion point $\mathbf{a} = \mathbf{0}$.

$$\tilde{f}_{\text{extrm}} = \tilde{f}(\check{\mathbf{x}}) = f(\mathbf{a}) + \frac{1}{2} \cdot \nabla_f^\top(\mathbf{a}) \cdot (\check{\mathbf{x}} - \mathbf{a}). \quad (\text{C.64})$$

Note that \tilde{f}_{extrm} may be a local minimum or maximum, but could also be a *saddle point* where the first derivatives of the function are zero as well.

Local extrema in 2D

The aforementioned scheme can be applied to n -dimensional functions. In the special case of a 2D function $f: \mathbb{R}^2 \mapsto \mathbb{R}$ (e.g., a 2D image), the gradient vector and the Hessian matrix for the given expansion point $\mathbf{a} = (x_a, y_a)^\top$ can be noted as

$$\nabla_f(\mathbf{a}) = \begin{pmatrix} d_x \\ d_y \end{pmatrix} \quad \text{and} \quad \mathbf{H}_f(\mathbf{a}) = \begin{pmatrix} H_{00} & H_{01} \\ H_{01} & H_{11} \end{pmatrix}, \quad (\text{C.65})$$

for a given expansion point $\mathbf{a} = (x_a, y_a)^\top$. In this case, the inverse of the Hessian matrix is

$$\mathbf{H}_f^{-1} = \frac{1}{H_{01}^2 - H_{00} \cdot H_{11}} \cdot \begin{pmatrix} -H_{11} & H_{01} \\ H_{01} & -H_{00} \end{pmatrix} \quad (\text{C.66})$$

and the resulting *position* of the extremal point is (see Eqn. (C.62))

$$\check{\mathbf{x}} = \begin{pmatrix} x_a \\ y_a \end{pmatrix} - \frac{1}{H_{01}^2 - H_{00} \cdot H_{11}} \cdot \begin{pmatrix} -H_{11} & H_{01} \\ H_{01} & -H_{00} \end{pmatrix} \cdot \begin{pmatrix} d_x \\ d_y \end{pmatrix} \quad (\text{C.67})$$

$$= \begin{pmatrix} x_a \\ y_a \end{pmatrix} - \frac{1}{H_{01}^2 - H_{00} \cdot H_{11}} \cdot \begin{pmatrix} H_{01} \cdot d_y - H_{11} \cdot d_x \\ H_{01} \cdot d_x - H_{00} \cdot d_y \end{pmatrix}. \quad (\text{C.68})$$

The extremal position is only defined if the denominator in Eqn. (C.68), $H_{01}^2 - H_{00} \cdot H_{11}$ (equivalent to the determinant of \mathbf{H}_f), is non-zero, indicating that the Hessian matrix \mathbf{H}_f is non-singular and thus has an inverse. The associated *value* of f at the estimated extremal position $\check{\mathbf{x}} = (\check{x}, \check{y})^\top$ can be now calculated using Eqn. (C.64) as

$$\begin{aligned} \tilde{f}(\check{x}, \check{y}) &= f(x_a, y_a) + \frac{1}{2} \cdot (d_x, d_y) \cdot \begin{pmatrix} \check{x} - x_a \\ \check{y} - y_a \end{pmatrix} \\ &= f(x_a, y_a) + \frac{d_x \cdot (\check{x} - x_a) + d_y \cdot (\check{y} - y_a)}{2}. \end{aligned} \quad (\text{C.69})$$

Numeric 2D example

The following example shows how a local extremum can be found in a discrete 2D image with sub-pixel accuracy using a second-order Taylor approximation. Assume we are given a grayscale image $I: \mathbb{Z} \times \mathbb{Z} \mapsto \mathbb{R}$ with the sample values

$$\begin{array}{ccc} & u_a-1 & u_a & u_a+1 \\ v_a-1 & 8 & 11 & 7 \\ v_a & 15 & 16 & 9 \\ v_a+1 & 14 & 12 & 10 \end{array} \quad (\text{C.70})$$

in the 3×3 neighborhood of position $\mathbf{a} = (u_a, v_a)^\top$. Obviously, the discrete center value $f(\mathbf{a}) = 16$ is a local maximum but (as we shall see) the maximum of the *continuous* approximation function is *not* at the center. The gradient vector ∇_I and the Hessian Matrix \mathbf{H}_I at the expansion point \mathbf{a} are calculated from local finite differences (see Sec. C.3.1) as

$$\nabla_I(\mathbf{a}) = \begin{pmatrix} d_x \\ d_y \end{pmatrix} = 0.5 \cdot \begin{pmatrix} 9-15 \\ 12-11 \end{pmatrix} = \begin{pmatrix} -3 \\ 0.5 \end{pmatrix} \quad \text{and} \quad (\text{C.71})$$

$$\begin{aligned} \mathbf{H}_I(\mathbf{a}) &= \begin{pmatrix} H_{11} & H_{12} \\ H_{12} & H_{22} \end{pmatrix} = \begin{pmatrix} 9-2 \cdot 16+15 & 0.25 \cdot (8-14-7+10) \\ 0.25 \cdot (8-14-7+10) & 11-2 \cdot 16+12 \end{pmatrix} \\ &= \begin{pmatrix} -8.00 & -0.75 \\ -0.75 & -9.00 \end{pmatrix}, \end{aligned} \quad (\text{C.72})$$

respectively. The resulting second-order Taylor expansion about the point \mathbf{a} is the continuous function (see Eqn. (C.52))

$$\begin{aligned} \tilde{f}(\mathbf{x}) &= f(\mathbf{a}) + \nabla_I^\top(\mathbf{a}) \cdot (\mathbf{x} - \mathbf{a}) + \frac{1}{2} \cdot (\mathbf{x} - \mathbf{a})^\top \cdot \mathbf{H}_I(\mathbf{a}) \cdot (\mathbf{x} - \mathbf{a}) \\ &= 16 + (-3, 0.5) \cdot \begin{pmatrix} x - u_a \\ y - v_a \end{pmatrix} \\ &\quad + \frac{1}{2} \cdot (x - u_a, y - v_a) \cdot \begin{pmatrix} -8.00 & -0.75 \\ -0.75 & -9.00 \end{pmatrix} \cdot \begin{pmatrix} x - u_a \\ y - v_a \end{pmatrix}. \end{aligned} \quad (\text{C.73})$$

We use the inverse of the 2×2 Hessian matrix at position \mathbf{a} (see Eqn. (C.66)),

$$\mathbf{H}_I^{-1}(\mathbf{a}) = \begin{pmatrix} -8.00 & -0.75 \\ -0.75 & -9.00 \end{pmatrix}^{-1} = \begin{pmatrix} -0.125984 & 0.010499 \\ 0.010499 & -0.111986 \end{pmatrix}, \quad (\text{C.74})$$

to calculate the *position* of the local extremum $\check{\mathbf{x}}$ (see Eqn. (C.68)) as

$$\begin{aligned} \check{\mathbf{x}} &= \mathbf{a} - \mathbf{H}_I^{-1}(\mathbf{a}) \cdot \nabla_I(\mathbf{a}) \\ &= \begin{pmatrix} u_a \\ v_a \end{pmatrix} - \begin{pmatrix} -0.125984 & 0.010499 \\ 0.010499 & -0.111986 \end{pmatrix} \cdot \begin{pmatrix} -3 \\ 0.5 \end{pmatrix} = \begin{pmatrix} u_a - 0.3832 \\ v_a + 0.0875 \end{pmatrix}. \end{aligned} \quad (\text{C.75})$$

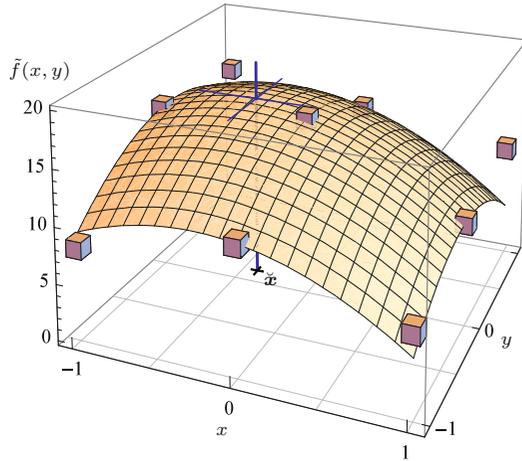
Finally, the extremal *value* (see Eqn. (C.64)) is found as

$$\begin{aligned} \tilde{f}(\check{\mathbf{x}}) &= f(\mathbf{a}) + \frac{1}{2} \cdot \nabla_f^T(\mathbf{a}) \cdot (\check{\mathbf{x}} - \mathbf{a}) \\ &= 16 + \frac{1}{2} \cdot (-3, 0.5) \cdot \begin{pmatrix} u_a - 0.3832 - u_a \\ v_a + 0.0875 - v_a \end{pmatrix} \\ &= 16 + \frac{1}{2} \cdot (3 \cdot 0.3832 + 0.5 \cdot 0.0875) = 16.5967. \end{aligned} \quad (\text{C.76})$$

Figure (C.3) illustrates the aforementioned example, with the expansion point set to $\mathbf{a} = (u_a, v_a)^T = (0, 0)^T$.

Fig. C.3

Continuous Taylor approximation of a discrete 2D image function for determining the local extremum position with sub-pixel accuracy. The cubes represent the discrete image samples in a 3×3 neighborhood around the reference coordinate $(0, 0)$, which is a local maximum of the discrete image function (see Eqn. (C.70) for the concrete values). The parabolic surface shows the continuous approximation $\tilde{f}(x, y)$ obtained by second-order Taylor expansion about the center position $\mathbf{a} = (0, 0)$. The vertical line marks the position of the local maximum $\tilde{f}(\check{\mathbf{x}}) = 16.5967$ at $\check{\mathbf{x}} = (-0.3832, 0.0875)$.



Local extrema in 3D

In the case of a three-variable, scalar function $f: \mathbb{R}^3 \mapsto \mathbb{R}$, with a given expansion point $\mathbf{a} = (x_a, y_a, z_a)^T$ and

$$\nabla_f(\mathbf{a}) = \begin{pmatrix} d_x \\ d_y \\ d_z \end{pmatrix} \quad \text{and} \quad \mathbf{H}_f(\mathbf{a}) = \begin{pmatrix} H_{00} & H_{01} & H_{02} \\ H_{01} & H_{11} & H_{12} \\ H_{02} & H_{12} & H_{22} \end{pmatrix} \quad (\text{C.77})$$

being the gradient vector and the Hessian matrix of f at point \mathbf{a} , respectively, the estimated extremal *position* is

$$\check{\mathbf{x}} = (\check{x}, \check{y}, \check{z})^\top = \mathbf{a} - \mathbf{H}_f^{-1}(\mathbf{a}) \cdot \nabla_f(\mathbf{a}) \quad (\text{C.78})$$

$$= \begin{pmatrix} x_a \\ y_a \\ z_a \end{pmatrix} - \frac{1}{H_{02}^2 \cdot H_{11} + H_{01}^2 \cdot H_{22} + H_{00} \cdot H_{12}^2 - H_{00} \cdot H_{11} \cdot H_{22} - 2 \cdot H_{01} \cdot H_{02} \cdot H_{12}} \cdot \begin{pmatrix} H_{12}^2 - H_{11} \cdot H_{22} & H_{01} \cdot H_{22} - H_{02} \cdot H_{12} & H_{02} \cdot H_{11} - H_{01} \cdot H_{12} \\ H_{01} \cdot H_{22} - H_{02} \cdot H_{12} & H_{02}^2 - H_{00} \cdot H_{22} & H_{00} \cdot H_{12} - H_{01} \cdot H_{02} \\ H_{02} \cdot H_{11} - H_{01} \cdot H_{12} & H_{00} \cdot H_{12} - H_{01} \cdot H_{02} & H_{01}^2 - H_{00} \cdot H_{11} \end{pmatrix} \cdot \begin{pmatrix} d_x \\ d_y \\ d_z \end{pmatrix}.$$

C.3 OPERATIONS ON MULTI-VARIABLE, SCALAR FUNCTIONS (SCALAR FIELDS)

Note that the inverse of the 3×3 Hessian matrix \mathbf{H}_f^{-1} is again symmetric and can be calculated in closed form (as shown in Eqn. (C.78)).⁴

Again using Eqn. (C.64), the estimated extremal *value* at position $\check{\mathbf{x}} = (\check{x}, \check{y}, \check{z})^\top$ is found as

$$\tilde{f}(\check{\mathbf{x}}) = f(\mathbf{a}) + \frac{1}{2} \cdot \nabla_f^\top(\mathbf{a}) \cdot (\check{\mathbf{x}} - \mathbf{a}) \quad (\text{C.79})$$

$$= f(\mathbf{a}) + \frac{d_x \cdot (\check{x} - x_a) + d_y \cdot (\check{y} - y_a) + d_z \cdot (\check{z} - z_a)}{2}. \quad (\text{C.80})$$

⁴ Nevertheless, the use of standard numerical methods is recommended.

Appendix D

Statistical Prerequisites

This part summarizes some essential statistical concepts for vector-valued data, intended as a supplement particularly to Chapters 11 and 17.

D.1 Mean, Variance, and Covariance

For the following definitions we assume a sequence $X = (\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_{n-1})$ of n vector-valued, m -dimensional measurements, with “samples”

$$\mathbf{x}_i = (x_{i,0}, x_{i,1}, \dots, x_{i,m-1})^\top \in \mathbb{R}^m. \quad (\text{D.1})$$

D.1.1 Mean

The n -dimensional *sample mean vector* is defined as

$$\boldsymbol{\mu}(X) = (\mu_0, \mu_1, \dots, \mu_{m-1})^\top \quad (\text{D.2})$$

$$= \frac{1}{n} \cdot (\mathbf{x}_0 + \mathbf{x}_1 + \dots + \mathbf{x}_{n-1}) = \frac{1}{n} \cdot \sum_{i=0}^{n-1} \mathbf{x}_i. \quad (\text{D.3})$$

Geometrically speaking, the vector $\boldsymbol{\mu}(X)$ corresponds to the *centroid* of the sample vectors \mathbf{x}_i in m -dimensional space. Each scalar element μ_p is the mean of the associated component (also called *variate* or *dimension*) p over all n samples, that is

$$\mu_p = \frac{1}{n} \cdot \sum_{i=0}^{n-1} x_{i,p}, \quad (\text{D.4})$$

for $p = 0, \dots, m-1$.

D.1.2 Variance and Covariance

The *covariance* quantifies the strength of interaction between a pair of components p, q in the sample X , defined as

$$\sigma_{p,q}(X) = \frac{1}{n} \cdot \sum_{i=0}^{n-1} (x_{i,p} - \mu_p) \cdot (x_{i,q} - \mu_q). \quad (\text{D.5})$$

For efficient calculation, this expression can be rewritten in the form

$$\sigma_{p,q}(X) = \frac{1}{n} \cdot \left[\underbrace{\sum_{i=0}^{n-1} (x_{i,p} \cdot x_{i,q})}_{S_{p,q}(X)} - \frac{1}{n} \cdot \left(\underbrace{\sum_{i=0}^{n-1} x_{i,p}}_{S_p(X)} \cdot \underbrace{\sum_{i=0}^{n-1} x_{i,q}}_{S_q(X)} \right) \right], \quad (\text{D.6})$$

which does not require the explicit calculation of μ_p and μ_q . In the special case of $p = q$, we get

$$\sigma_{p,p}(X) = \sigma_p^2(X) = \frac{1}{n} \cdot \sum_{i=0}^{n-1} (x_{i,p} - \mu_p)^2 \quad (\text{D.7})$$

$$= \frac{1}{n} \cdot \left[\sum_{i=0}^{n-1} x_{i,p}^2 - \frac{1}{n} \cdot \left(\sum_{i=0}^{n-1} x_{i,p} \right)^2 \right], \quad (\text{D.8})$$

which is the *variance within* the component p . This corresponds to the ordinary (one-dimensional) variance $\sigma_p^2(X)$ of the n scalar sample values $x_{0,p}, x_{1,p}, \dots, x_{n-1,p}$ (see also Sec. 3.7.1).

D.1.3 Biased vs. Unbiased Variance

If the variance (or covariance) of some population is estimated from a small set of random samples, the results obtained by the formulation given in the previous section are known to be statistically *biased*.¹ The most common form of correcting for this bias is to use the factor $1/(n-1)$ instead of $1/n$ in the variance calculations. For example, Eqn. (D.5) would change to

$$\check{\sigma}_{p,q}(X) = \frac{1}{n-1} \cdot \sum_{i=0}^{n-1} (x_{i,p} - \mu_p) \cdot (x_{i,q} - \mu_q) \quad (\text{D.9})$$

to yield an *unbiased* sample variance. In the following (and throughout the text), we ignore the bias issue and consistently use the factor $1/n$ for all variance calculations. Note, however, that many software packages² use the bias-corrected factor $1/(n-1)$ by default and thus may return different results (which can be easily scaled for comparison).

D.2 The Covariance Matrix

The *covariance matrix* Σ for the m -dimensional sample X is a square matrix of size $m \times m$ that is composed of the covariance values $\sigma_{p,q}$ for all pairs (p, q) of components, that is,

¹ Note that the estimation of the mean by the *sample mean* (Eqn. (D.3)) is not affected by this bias problem.

² For example, *Apache Commons Math*, *Matlab*, *Mathematica*.

$$\Sigma(X) = \begin{pmatrix} \sigma_{0,0} & \sigma_{0,1} & \cdots & \sigma_{0,m-1} \\ \sigma_{1,0} & \sigma_{1,1} & \cdots & \sigma_{1,m-1} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{m-1,0} & \sigma_{m-1,1} & \cdots & \sigma_{m-1,m-1} \end{pmatrix} \quad (\text{D.10})$$

$$= \begin{pmatrix} \sigma_0^2 & \sigma_{0,1} & \cdots & \sigma_{0,m-1} \\ \sigma_{1,0} & \sigma_1^2 & \cdots & \sigma_{1,m-1} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{m-1,0} & \sigma_{m-1,1} & \cdots & \sigma_{m-1}^2 \end{pmatrix}. \quad (\text{D.11})$$

Note that any diagonal element of $\Sigma(X)$ is the ordinary (scalar) variance $\sigma_p^2(X)$ (see Eqn. (D.7)), for $p = 0, \dots, m-1$, which can never be negative. All other entries of a covariance matrix may be positive or negative in general. Since $\sigma_{p,q} = \sigma_{q,p}$, a covariance matrix is always symmetric, with up to $(m^2 + m)/2$ unique elements. Thus, any covariance matrix has the important property of being *positive semidefinite*, which implies that all its eigenvalues (see Sec. B.4) are positive (i.e., non-negative). The covariance matrix can also be written in the form

$$\Sigma(X) = \frac{1}{n} \cdot \sum_{i=0}^{n-1} \underbrace{[\mathbf{x}_i - \boldsymbol{\mu}(X)] \cdot [\mathbf{x}_i - \boldsymbol{\mu}(X)]^\top}_{= [\mathbf{x}_i - \boldsymbol{\mu}(X)] \otimes [\mathbf{x}_i - \boldsymbol{\mu}(X)]}, \quad (\text{D.12})$$

where \otimes denotes the outer (vector) product.

The *trace* (sum of the diagonal elements) of the covariance matrix,

$$\sigma_{\text{total}}(X) = \text{trace}(\Sigma(X)), \quad (\text{D.13})$$

is called the *total variance* of the multivariate sample. Alternatively, the (Frobenius) *norm* of the covariance matrix $\Sigma(X)$, defined as

$$\|\Sigma(X)\|_2 = \left(\sum_{i=0}^{m-1} \sum_{j=0}^{m-1} \sigma_{i,j}^2 \right)^{1/2}, \quad (\text{D.14})$$

can be used to quantify the overall variance in the sample data.

D.2.1 Example

Assume that the sample X consists of the following set of four 3D vectors (i.e., $m = 3$ and $n = 4$)

$$\mathbf{x}_0 = \begin{pmatrix} 75 \\ 37 \\ 12 \end{pmatrix}, \quad \mathbf{x}_1 = \begin{pmatrix} 41 \\ 27 \\ 20 \end{pmatrix}, \quad \mathbf{x}_2 = \begin{pmatrix} 93 \\ 81 \\ 11 \end{pmatrix}, \quad \mathbf{x}_3 = \begin{pmatrix} 12 \\ 48 \\ 52 \end{pmatrix},$$

with each $\mathbf{x}_i = (x_{i,R}, x_{i,G}, x_{i,B})^\top$ representing a particular RGB color. The resulting *sample mean vector* (see Eqn. (D.3)) is

$$\boldsymbol{\mu}(X) = \begin{pmatrix} \mu_R \\ \mu_G \\ \mu_B \end{pmatrix} = \frac{1}{4} \cdot \begin{pmatrix} 75 + 41 + 93 + 12 \\ 37 + 27 + 81 + 48 \\ 12 + 20 + 11 + 52 \end{pmatrix} = \frac{1}{4} \cdot \begin{pmatrix} 221 \\ 193 \\ 95 \end{pmatrix} = \begin{pmatrix} 55.25 \\ 48.25 \\ 23.75 \end{pmatrix},$$

and the associated *covariance matrix* (Eqn. (D.11)) is

$$\Sigma(X) = \begin{pmatrix} 972.188 & 331.938 & -470.438 \\ 331.938 & 412.688 & -53.188 \\ -470.438 & -53.188 & 278.188 \end{pmatrix}.$$

As predicted, this matrix is symmetric and all diagonal elements are non-negative. Note that *no* sample bias-correction (see Sec. D.1.3) was used in this example. The *total variance* (Eqn. (D.13)) of the sample set is

$$\sigma_{\text{total}}(X) = \text{trace}(\Sigma(X)) = 972.188 + 412.688 + 278.188 \approx 1663.06,$$

and the *Froebenius norm* of the covariance matrix (see Eqn. (D.14)) is $\|\Sigma(X)\|_2 \approx 1364.36$.

D.2.2 Practical Calculation

The calculation of covariance matrices is implemented in almost any software package for statistical analysis or linear algebra. For example, with the *Apache Commons Math* library this could be accomplished as follows:

```
import org.apache.commons.math3.stat.correlation.Covariance;
...
double[][] X;          // X[i] is the i-th sample vector
Covariance cov = new Covariance(X, false); // no bias correction
RealMatrix S = cov.getCovarianceMatrix();
...
```

D.3 Mahalanobis Distance

The Mahalanobis distance³ [157] is used to measure distances in multi-dimensional distributions. Unlike the Euclidean distance it takes into account the amount of scatter in the distribution and the correlation between features. In particular, the Mahalanobis distance can be used to measure distances in distributions, where the individual components substantially differ in scale. Depending on their scale, a few components (or even a single component) may dominate the ordinary (Euclidean) distance outcome and the “smaller” components have no influence whatsoever.

D.3.1 Definition

Given a distribution of m -dimensional samples $X = (\mathbf{x}_0, \dots, \mathbf{x}_{n-1})$, with $\mathbf{x}_k \in \mathbb{R}^m$, the Mahalanobis distance between two samples \mathbf{x}_a , \mathbf{x}_b is defined as

$$d_M(\mathbf{x}_a, \mathbf{x}_b) = \|\mathbf{x}_a - \mathbf{x}_b\|_M = \sqrt{(\mathbf{x}_a - \mathbf{x}_b)^\top \cdot \Sigma^{-1} \cdot (\mathbf{x}_a - \mathbf{x}_b)}, \quad (\text{D.15})$$

where Σ is the $m \times m$ *covariance matrix* of the distribution X , as described in Sec. D.2.⁴

³ http://en.wikipedia.org/wiki/Mahalanobis_distance.

⁴ Note that the expression under the root in Eqn. (D.15) is the (dot) product of a row vector and a column vector, that is, the result is a non-negative scalar value.

The Mahalanobis distance normalizes each feature component to *zero mean* and *unit variance*. This makes the distance calculation independent of the scale of the individual components, that is, all components are “treated fairly” even if their range is many orders of magnitude different. In other words, no component can dominate the others even if its magnitude is disproportionately large.

D.3.2 Relation to the Euclidean Distance

Recall that the Euclidean distance between two points $\mathbf{x}_a, \mathbf{x}_b$ in \mathbb{R}^m is equivalent to the (L2) norm of the difference vector $\mathbf{x}_a - \mathbf{x}_b$, which can be written in the form

$$d_E(\mathbf{x}_a, \mathbf{x}_b) = \|\mathbf{x}_a - \mathbf{x}_b\|_2 = \sqrt{(\mathbf{x}_a - \mathbf{x}_b)^\top \cdot (\mathbf{x}_a - \mathbf{x}_b)}. \quad (\text{D.16})$$

Note the structural similarity with the definition of the Mahalanobis distance in Eqn. (D.15), the only difference being the missing matrix Σ^{-1} . This becomes even clearer if we analogously insert the identity matrix \mathbf{I} into Eqn. (D.16), that is,

$$d_E(\mathbf{x}_a, \mathbf{x}_b) = \|\mathbf{x}_a - \mathbf{x}_b\|_2 = \sqrt{(\mathbf{x}_a - \mathbf{x}_b)^\top \cdot \mathbf{I} \cdot (\mathbf{x}_a - \mathbf{x}_b)}, \quad (\text{D.17})$$

which obviously does not change the outcome. The purpose of Σ^{-1} in Eqn. (D.15) is to map the difference vectors (and thus the involved vectors $\mathbf{x}_a, \mathbf{x}_b$) into a transformed (scaled and rotated) space, where the actual distance measurement is performed. In contrast, with the Euclidean distance, all components contribute equally to the distance measure, without any scaling or other transformation.

D.3.3 Numerical Aspects

For calculating the Mahalanobis distance (Eqn. (D.15)) the *inverse* of the covariance matrix (Sec. D.2) is needed. By definition, a covariance matrix Σ is symmetric and its diagonal values are non-negative. Similarly (at least in theory), its inverse Σ^{-1} should also be symmetric with non-negative diagonal values. This is necessary to ensure that the quantities under the square root in Eqn. (D.15) are always positive.

Unfortunately, Σ is often ill-conditioned because of diagonal values that are very small or even zero. In this case, Σ is not positive-definite (as it should be), that is, one or more of its eigenvalues are negative, the inversion becomes numerically unstable and the resulting Σ^{-1} is non-symmetric. A simple remedy to this problem is to add a small quantity to the diagonal of the original covariance matrix Σ , that is,

$$\tilde{\Sigma} = \Sigma + \epsilon \cdot \mathbf{I}, \quad (\text{D.18})$$

to enforce positive definiteness, and to use $\tilde{\Sigma}^{-1}$ in Eqn. (D.15).

A possible alternative is to calculate the *Eigen decomposition*⁵ of Σ in the form

⁵ See <http://mathworld.wolfram.com/EigenDecomposition.html> and the class `EigenDecomposition` in the *Apache Commons Math* library.

$$\Sigma = \mathbf{V} \cdot \mathbf{\Lambda} \cdot \mathbf{V}^T \quad (\text{D.19})$$

where $\mathbf{\Lambda}$ is a diagonal matrix containing the eigenvalues of Σ (which may be zero or negative). From this we create a modified diagonal matrix $\tilde{\mathbf{\Lambda}}$ by substituting all non-positive eigenvalues with a small positive quantity ϵ , that is,

$$\tilde{\Lambda}_{i,i} = \min(\Lambda_{i,i}, \epsilon). \quad (\text{D.20})$$

(typically $\epsilon \approx 10^{-6}$) and finally calculate the modified covariance matrix as

$$\tilde{\Sigma} = \mathbf{V} \cdot \tilde{\mathbf{\Lambda}} \cdot \mathbf{V}^T, \quad (\text{D.21})$$

which should be positive definite. The (symmetric) inverse $\tilde{\Sigma}^{-1}$ is then used in Eqn. (D.15).

D.3.4 Pre-Mapping Data for Efficient Mahalanobis Matching

Assume that we have a large set of sample vectors (“data base”) $X = (\mathbf{x}_0, \dots, \mathbf{x}_{n-1})$ which shall be frequently queried for the instance most similar (i.e., closest) to a given search sample \mathbf{x}_s . Assuming that the search through X is performed linearly, we would need to calculate $d_M(\mathbf{x}_s, \mathbf{x}_i)$ —using Eqn. (D.15)—for all elements of \mathbf{x}_i in X .

One way to accelerate the matching is to perform the transformation defined by Σ^{-1} to the entire data set only once, such that the Euclidean norm alone can be used for the distance calculation. For the sake of simplicity we write

$$d_M^2(\mathbf{x}_a, \mathbf{x}_b) = \|\mathbf{x}_a - \mathbf{x}_b\|_M^2 = \|\mathbf{y}\|_M^2 \quad (\text{D.22})$$

with the difference vector $\mathbf{y} = \mathbf{x}_a - \mathbf{x}_b$, such that Eqn. (D.15) becomes

$$\|\mathbf{y}\|_M^2 = \mathbf{y}^T \cdot \Sigma^{-1} \cdot \mathbf{y}. \quad (\text{D.23})$$

The goal is to find a transformation \mathbf{U} such that we can calculate the Mahalanobis distance from the transformed vectors directly as

$$\hat{\mathbf{y}} = \mathbf{U} \cdot \mathbf{y}, \quad (\text{D.24})$$

by using the ordinary *Euclidean* norm $\|\cdot\|_2$ instead, that is, in the form

$$\|\mathbf{y}\|_M^2 = \|\hat{\mathbf{y}}\|_2^2 = \hat{\mathbf{y}}^T \cdot \hat{\mathbf{y}} \quad (\text{D.25})$$

$$= (\mathbf{U} \cdot \mathbf{y})^T \cdot (\mathbf{U} \cdot \mathbf{y}) = (\mathbf{y}^T \cdot \mathbf{U}^T) \cdot (\mathbf{U} \cdot \mathbf{y}) \quad (\text{D.26})$$

$$= \mathbf{y}^T \cdot \mathbf{U}^T \cdot \mathbf{U} \cdot \mathbf{y} = \mathbf{y}^T \cdot \Sigma^{-1} \cdot \mathbf{y}. \quad (\text{D.27})$$

While we do not know the matrix \mathbf{U} yet, we see from Eqn. (D.27) that it must satisfy

$$\mathbf{U}^T \cdot \mathbf{U} = \Sigma^{-1}. \quad (\text{D.28})$$

Fortunately, since Σ^{-1} is symmetric and positive definite, such a decomposition of Σ^{-1} always exists.

The standard method for calculating \mathbf{U} in Eqn. (D.28) is by the Cholesky decomposition,⁶ which can factorize any symmetric, positive definite matrix \mathbf{A} in the form

$$\mathbf{A} = \mathbf{L} \cdot \mathbf{L}^\top \quad \text{or} \quad \mathbf{A} = \mathbf{U}^\top \cdot \mathbf{U}, \quad (\text{D.29})$$

where \mathbf{L} is a *lower-triangular* matrix or, alternatively, \mathbf{U} is an *upper-triangular* matrix (the second variant is the one we need).⁷ Since the transformation of the difference vectors $\mathbf{y} \rightarrow \mathbf{U} \cdot \mathbf{y}$ is a linear operation, the result is the same if we apply the transformation individually to the original vectors, that is,

$$\hat{\mathbf{y}} = \mathbf{U} \cdot \mathbf{y} = \mathbf{U} \cdot (\mathbf{x}_a - \mathbf{x}_b) = \mathbf{U} \cdot \mathbf{x}_a - \mathbf{U} \cdot \mathbf{x}_b. \quad (\text{D.30})$$

This means that, given the transformation \mathbf{U} , we can obtain the Mahalanobis distance between two points $\mathbf{x}_a, \mathbf{x}_b$ (as defined in Eqn. (D.15)) by simply calculating the Euclidean distance in the form

$$d_M(\mathbf{x}_a, \mathbf{x}_b) = \|\mathbf{U} \cdot (\mathbf{x}_a - \mathbf{x}_b)\|_2 = \|\mathbf{U} \cdot \mathbf{x}_a - \mathbf{U} \cdot \mathbf{x}_b\|_2. \quad (\text{D.31})$$

In summary, this suggests the following solution to a large-database Mahalanobis matching problem:

1. Calculate the covariance matrix Σ for the original dataset $X = (\mathbf{x}_0, \dots, \mathbf{x}_{n-1})$.
2. Condition Σ , such that it is positive definite (see Sec. D.3.3).
3. Find the matrix \mathbf{U} , such that $\mathbf{U}^\top \cdot \mathbf{U} = \Sigma^{-1}$ (by Cholesky decomposition of Σ^{-1}).
4. Transform all samples of the original data set $X = (\mathbf{x}_0, \dots, \mathbf{x}_{n-1})$ to $\hat{X} = (\hat{\mathbf{x}}_0, \dots, \hat{\mathbf{x}}_{n-1})$, with $\hat{\mathbf{x}}_k = \mathbf{U} \cdot \mathbf{x}_k$. This now becomes the actual “database”.
5. Apply the same transformation to the search sample \mathbf{x}_s , that is, calculate $\hat{\mathbf{x}}_s = \mathbf{U} \cdot \mathbf{x}_s$.
6. Find the index l of the best-matching element in X (in terms of the Mahalanobis distance) by calculating the *Euclidean* (!) distance between the transformed vectors, that is

$$l = \underset{0 \leq k < n}{\operatorname{argmin}} \|\hat{\mathbf{x}}_s - \hat{\mathbf{x}}_k\|^2. \quad (\text{D.32})$$

Since the matching is now performed with the ordinary Euclidean distance and the Mahalanobis calculation is not required during the search, the savings should be substantial. Also, this opens an easy path to the use of advanced, tree-based matching techniques, such as the common k -nearest neighbor methods.

⁶ See <http://mathworld.wolfram.com/CholeskyDecomposition.html>.

⁷ The Cholesky decomposition (CD) requires that the supplied matrix \mathbf{A} is symmetric and positive definite, otherwise the decomposition will fail. In fact, the CD itself is commonly used to test if a given matrix is positive definite. It is implemented by class `CholeskyDecomposition` of the *Apache Commons Math* library.

D.4 The Gaussian Distribution

The Gaussian distribution plays a major role in decision theory, pattern recognition, and statistics in general, because of its convenient analytical properties. A continuous, scalar quantity X is said to be subject to a Gaussian distribution, if the probability of observing a particular value x is

$$p(X=x) = p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \cdot e^{-\frac{(x-\mu)^2}{2\cdot\sigma^2}}. \quad (\text{D.33})$$

The Gaussian distribution is completely defined by its mean μ and variance σ^2 . The Gaussian distribution, also called a “normal” distribution, is commonly denoted in the form

$$p(x) \sim \mathcal{N}(X|\mu, \sigma^2) \quad \text{or} \quad X \sim \mathcal{N}(\mu, \sigma^2), \quad (\text{D.34})$$

saying that “ X is normally distributed with parameters μ and σ^2 .” As required for any valid probability distribution,

$$\mathcal{N}(X|\mu, \sigma^2) > 0 \quad \text{and} \quad \int_{-\infty}^{\infty} \mathcal{N}(X|\mu, \sigma^2) dx = 1. \quad (\text{D.35})$$

Thus the area under the probability distribution curve is always one, that is, $\mathcal{N}()$ is normalized. The Gaussian function in Eqn. (D.33) has its maximum height (called “mode”) at position $x = \mu$, where its value is

$$p(x=\mu) = \frac{1}{\sqrt{2\pi\sigma^2}}. \quad (\text{D.36})$$

If a random variable X is normally distributed with mean μ and variance σ^2 , then the result of a linear mapping of the kind $X' = aX + b$ is again a random variable that is normally distributed, with parameters $\bar{\mu} = a\cdot\mu + b$ and $\bar{\sigma}^2 = a^2\cdot\sigma^2$:

$$X \sim \mathcal{N}(\mu, \sigma^2) \Rightarrow a\cdot X + b \sim \mathcal{N}(a\cdot\mu + b, a^2\cdot\sigma^2), \quad (\text{D.37})$$

for $a, b \in \mathbb{R}$.

Moreover, if X_1, X_2 are statistically *independent*, normally distributed random variables with means μ_1, μ_2 and variances σ_1^2, σ_2^2 , respectively, then a linear combination of the form $a_1X_1 + a_2X_2$ is again normally distributed with $\mu_{12} = a_1\cdot\mu_1 + a_2\cdot\mu_2$ and $\sigma_{12} = a_1^2\cdot\sigma_1^2 + a_2^2\cdot\sigma_2^2$, that is,

$$(a_1X_1 + a_2X_2) \sim \mathcal{N}(a_1\cdot\mu_1 + a_2\cdot\mu_2, a_1^2\cdot\sigma_1^2 + a_2^2\cdot\sigma_2^2). \quad (\text{D.38})$$

D.4.1 Maximum Likelihood Estimation

The probability density function $p(x)$ of a statistical distribution tells us how probable it is to observe the result x for some fixed distribution parameters, such as μ and σ , in case of a normal distribution. If these parameters are *unknown* and need to be estimated,⁸ it is interesting to ask the reverse question:

⁸ As required, for example, for “minimum error thresholding” in Chapter 11, Sec. 11.1.6.

How likely are particular parameter values for a given set of empirical observations (assuming a certain type of distribution)?

This is (in a casual sense) what the term “likelihood” stands for. In particular, a distribution’s *likelihood function* quantifies the probability that a given (fixed) set of observations was generated by some varying distribution parameters.

Note that the probability of observing the outcome x from the normal distribution,

$$p(x) = p(x | \mu, \sigma^2), \quad (\text{D.39})$$

is really a *conditional* probability, stating how probable it is to observe the value x from a given normal distribution with known parameters μ and σ^2 . Conversely, a likelihood function for the normal distribution could be viewed as a conditional function

$$L(\mu, \sigma^2 | x), \quad (\text{D.40})$$

which quantifies the likelihood of (μ, σ^2) being the correct distribution parameters for a given observation x . The maximum likelihood method tries to find optimal parameters by *maximizing* the value of a distribution’s likelihood function L .

If we draw two independent⁹ samples x_a, x_b that are subjected to the same distribution, their *joint probability* (i.e., the probability of x_a and x_b occurring together in the sample) is the product of their individual probabilities, that is,

$$p(x_a \wedge x_b) = p(x_a) \cdot p(x_b). \quad (\text{D.41})$$

In general, if we are given a vector of m independent observations $X = (x_1, x_2, \dots, x_m)$ from the same distribution, the probability of observing exactly this set of values is

$$\begin{aligned} p(X) &= p(x_0 \wedge x_1 \wedge \dots \wedge x_{m-1}) \\ &= p(x_0) \cdot p(x_1) \cdot \dots \cdot p(x_{m-1}) = \prod_{i=0}^{m-1} p(x_i). \end{aligned} \quad (\text{D.42})$$

Thus, if the sample X originates from a normal distribution \mathcal{N} , a suitable likelihood function is

$$L(\mu, \sigma^2 | X) = p(X | \mu, \sigma^2) \quad (\text{D.43})$$

$$= \prod_{i=0}^{m-1} \mathcal{N}(x_i | \mu, \sigma^2) = \prod_{i=0}^{m-1} \frac{1}{\sqrt{2\pi\sigma^2}} \cdot e^{-\frac{(x_i - \mu)^2}{2 \cdot \sigma^2}}. \quad (\text{D.44})$$

The parameters $(\hat{\mu}, \hat{\sigma}^2)$, for which $L(\mu, \sigma^2 | X)$ is a maximum, are called the maximum-likelihood estimate for X .

Note that it is not necessary for a likelihood function to be a proper (i.e., normalized) probability distribution, since it is only necessary to calculate whether a particular set of distribution parameters

⁹ Although this assumption is often violated, independence is important to keep statistical problems simple and tractable. In particular, the values of adjacent image pixels are usually not independent.

is more probable than another. Thus the likelihood function L may be any monotonic function of the corresponding probability p in Eqn. (D.43), in particular its *logarithm*, which is commonly used to avoid multiplying small values.

D.4.2 Gaussian Mixtures

In practice, probabilistic models are often too complex to be described by a single Gaussian (or other standard) distribution. Without losing the mathematical convenience of Gaussian models, highly complex distributions can be modeled as combinations of multiple Gaussian distributions with different parameters. Such a Gaussian *mixture model* is a linear superposition of K Gaussian distributions of the form

$$p(x) = \sum_{j=0}^{K-1} \pi_j \cdot \mathcal{N}(x | \mu_j, \sigma_j^2), \quad (\text{D.45})$$

where the weights (“mixing coefficients”) π_j express the probability that an event x was generated by the j^{th} component (with $\sum_{j=0}^{K-1} \pi_j = 1$).¹⁰ The interpretation of this mixture model is, that there are K independent Gaussian “components” (each with its parameters μ_j, σ_j) that contribute to a common stream of events x_i . If a particular value x is observed, it is assumed to be the result of exactly *one* of the K components, but the identity of that component is unknown.

Assume, as a special case, that a probability distribution $p(x)$ is the superposition (mixture) of *two* Gaussian distributions, that is,

$$p(x) = \pi_a \cdot \mathcal{N}(x | \mu_a, \sigma_a^2) + \pi_b \cdot \mathcal{N}(x | \mu_b, \sigma_b^2). \quad (\text{D.46})$$

Any observed value x is assumed to be generated by either the first component (with μ_a, σ_a^2 and prior probability π_a) or the second component (with μ_b, σ_b^2 and prior probability π_b). These parameters as well as the prior probabilities are unknown but can be estimated by maximizing the likelihood function L . Note that, in general, the unknown parameters cannot be calculated in closed form but only with numerical methods. For further details and solution techniques see [24, 64, 228], for example.

D.4.3 Creating Gaussian Noise

Synthetic Gaussian noise is often used for testing in image processing, particularly for assessing the quality of smoothing filters. While the generation of pseudo-random values that follow a Gaussian distribution is not a trivial task in general,¹¹ it is readily implemented in Java by the standard class `Random`. For example, the Java method `addGaussianNoise()` in Prog. D.1 adds Gaussian noise with zero mean ($\mu = 0$) and standard deviation `sigma` (σ) to a grayscale image `I` of type `FloatProcessor` (`ImageJ`). The random values produced

¹⁰ The weight π_j is also called the *prior* probability of the component j .

¹¹ Typically the so-called *polar method* is used for generating Gaussian random values [138, Sec. 3.4.1].

by successive calls to the method `nextGaussian()` in line 10 follow a Gaussian distribution $\mathcal{N}(0, 1)$, with mean $\mu = 0$ and variance $\sigma^2 = 1$. As implied by Eqn. (D.37),

$$X \sim \mathcal{N}(0, 1) \Rightarrow a + s \cdot X \sim \mathcal{N}(a, s^2), \quad (\text{D.47})$$

and thus scaling the results from `nextGaussian()` by `s` and additive shifting by `a` makes the resulting random variable `noise` normally distributed with $\mathcal{N}(a, s^2)$.

D.4 THE GAUSSIAN DISTRIBUTION

Prog. D.1

Java method for adding Gaussian noise to an image of type `FloatProcessor`.

```
1 import java.util.Random;
2
3 void addGaussianNoise (FloatProcessor I, double sigma) {
4     int w = I.getWidth();
5     int h = I.getHeight();
6     Random rnd = new Random();
7     for (int v = 0; v < h; v++) {
8         for (int u = 0; u < w; u++) {
9             float val = I.getf(u, v);
10            float noise = (float) (rnd.nextGaussian() * sigma);
11            I.setf(u, v, val + noise);
12        }
13    }
14 }
```

Appendix E

Gaussian Filters

This part supplements the material presented in Ch. 25 (SIFT).

E.1 Cascading Gaussian Filters

To compute a Gaussian scale space efficiently (as used in the SIFT method, for example), the scale layers are usually not obtained directly from the input image by smoothing with Gaussians of increasing size. Instead, each layer can be calculated recursively from the previous layer by filtering with relatively small Gaussians. Thus, the entire scale space is implemented as a concatenation or “cascade” of smaller Gaussian filters.¹

If Gaussian filters of sizes σ_1, σ_2 are applied successively to the same image, the resulting smoothing effect is identical to using a single larger Gaussian filter H_σ^G , that is,

$$(I * H_{\sigma_1}^G) * H_{\sigma_2}^G = I * (H_{\sigma_1}^G * H_{\sigma_2}^G) = I * H_\sigma^G, \quad (\text{E.1})$$

with $\sigma = \sqrt{\sigma_1^2 + \sigma_2^2}$ being the size of the resulting combined Gaussian filter H_σ^G [129, Sec. 4.5.4]. Put in other words, the *variances* (squares of the σ values) of successive Gaussian filters add up, that is,

$$\sigma^2 = \sigma_1^2 + \sigma_2^2. \quad (\text{E.2})$$

In the special case of the *same* Gaussian filter being applied twice ($\sigma_1 = \sigma_2$), the effective width of the combined filter is $\sigma = \sqrt{2} \cdot \sigma_1$.

E.2 Gaussian Filters and Scale Space

In a Gaussian scale space, the scale corresponding to each level is proportional to the width (σ) of the Gaussian filter required to derive this level from the original (completely unsmoothed) image. Given an image that is already pre-smoothed by a Gaussian filter of width

¹ See Chapter 25, Sec. 25.1.1 for details.

σ_1 and should be smoothed to some target scale $\sigma_2 > \sigma_1$, the required width of the additional Gaussian filter is

$$\sigma_d = \sqrt{\sigma_2^2 - \sigma_1^2}. \quad (\text{E.3})$$

Usually the neighboring layers of the scale space differ by a constant scale factor (κ) and the transformation from one scale level to another can be accomplished by successively applying Gaussian filters. Despite the constant scale factor, however, the width of the required filters is *not* constant but depends on the image's initial scale. In particular, if we want to transform an image with scale σ_0 by a factor κ to a new scale $\kappa \cdot \sigma_0$, then (from Eqn. (E.2)) for σ_d the relation

$$(\kappa \cdot \sigma_0)^2 = \sigma_0^2 + \sigma_d^2 \quad (\text{E.4})$$

must hold. Thus, the width σ_d of the required Gaussian smoothing filter is

$$\sigma_d = \sigma_0 \cdot \sqrt{\kappa^2 - 1}. \quad (\text{E.5})$$

For example, doubling the scale ($\kappa = 2$) of an image that is pre-smoothed with σ_0 requires a Gaussian filter of width $\sigma_d = \sigma_0 \cdot (2^2 - 1)^{1/2} = \sigma_0 \cdot \sqrt{3} \approx \sigma_0 \cdot 1.732$.

E.3 Effects of Gaussian Filtering in the Frequency Domain

For the 1D Gaussian function

$$g_\sigma(x) = \frac{1}{\sigma\sqrt{2\pi}} \cdot e^{-\frac{x^2}{2\sigma^2}} \quad (\text{E.6})$$

the continuous Fourier transform² $\mathcal{F}(g_\sigma)$ is

$$G_\sigma(\omega) = \frac{1}{\sqrt{2\pi}} \cdot e^{-\frac{\omega^2\sigma^2}{2}}. \quad (\text{E.7})$$

Doubling the width (σ) of a Gaussian filter corresponds to cutting the bandwidth by half. If σ is doubled, the Fourier transform becomes

$$G_{2\sigma}(\omega) = \frac{1}{\sqrt{2\pi}} \cdot e^{-\frac{\omega^2(2\sigma)^2}{2}} = \frac{1}{\sqrt{2\pi}} \cdot e^{-\frac{4\omega^2\sigma^2}{2}} \quad (\text{E.8})$$

$$= \frac{1}{\sqrt{2\pi}} \cdot e^{-\frac{(2\omega)^2\sigma^2}{2}} = G_\sigma(2\omega) \quad (\text{E.9})$$

and, in general, when scaling the filter by a factor k ,

$$G_{k\sigma}(\omega) = G_\sigma(k\omega). \quad (\text{E.10})$$

That is, if σ is *increased* (or the kernel widened) by a factor k , the corresponding Fourier transform gets *contracted* by the same factor. In terms of linear filtering this means that widening the kernel by some factor k decimates the resulting signal bandwidth by $\frac{1}{k}$.

² See also Chapter 18, Sec. 18.1.

E.4 LoG-Approximation by the DoG

The 2D LoG kernel (see Ch. 25, Sec. 25.1.1),

$$L_\sigma(x, y) = (\nabla^2 g_\sigma)(x, y) = \frac{1}{\pi\sigma^4} \left(\frac{x^2 + y^2 - 2\sigma^2}{2\sigma^2} \right) \cdot e^{-\frac{x^2 + y^2}{2\sigma^2}}, \quad (\text{E.11})$$

has a (negative) peak at the origin with the associated function value

$$L_\sigma(0, 0) = -\frac{1}{\pi\sigma^4}. \quad (\text{E.12})$$

Thus, the *scale normalized* LoG kernel, defined in Eqn. (25.10) as

$$\hat{L}_\sigma(x, y) = \sigma^2 \cdot L_\sigma(x, y), \quad (\text{E.13})$$

has the peak value

$$\hat{L}_\sigma(0, 0) = -\frac{1}{\pi\sigma^2} \quad (\text{E.14})$$

at the origin. In comparison, for a given scale factor κ , the unscaled DoG function

$$\begin{aligned} \text{DoG}_{\sigma,\kappa}(x, y) &= G_{\kappa\sigma}(x, y) - G_\sigma(x, y) \\ &= \frac{1}{2\pi\kappa^2\sigma^2} \cdot e^{-\frac{x^2 + y^2}{2\kappa^2\sigma^2}} - \frac{1}{2\pi\sigma^2} \cdot e^{-\frac{x^2 + y^2}{2\sigma^2}}, \end{aligned} \quad (\text{E.15})$$

has a peak value

$$\text{DoG}_{\sigma,\kappa}(0, 0) = -\frac{\kappa^2 - 1}{2\pi\kappa^2\sigma^2}. \quad (\text{E.16})$$

By scaling the DoG function by some factor λ to match the LoG's center peak value, such that $L_\sigma(0, 0) = \lambda \cdot \text{DoG}_{\sigma,\kappa}(0, 0)$, the original LoG (Eqn. (E.11)) is approximated by the DoG in the form

$$L_\sigma(x, y) \approx \frac{2\kappa^2}{\sigma^2(\kappa^2 - 1)} \cdot \text{DoG}_{\sigma,\kappa}(x, y). \quad (\text{E.17})$$

Similarly, the scale-normalized LoG (Eqn. (E.13)) is approximated by the DoG as³

$$\hat{L}_\sigma(x, y) \approx \frac{2\kappa^2}{\kappa^2 - 1} \cdot \text{DoG}_{\sigma,\kappa}(x, y). \quad (\text{E.18})$$

Since the factor in Eqn. (E.18) depends on κ only, the DoG approximation is (for a constant size ratio κ) implicitly proportional to the scale normalized LoG for any scale σ .

³ A different formulation, $\hat{L}_\sigma(x, y) \approx \frac{1}{\kappa - 1} \cdot \text{DoG}_{\sigma,\kappa}(x, y)$, is given in [153], which is the same as Eqn. (E.18) for $\kappa \rightarrow 1$, but not for $\kappa > 1$. The essence is that the leading factor is constant and independent of σ , and can thus be ignored when comparing the magnitude of the filter responses at varying scales.

Appendix F

Java Notes

As a text for undergraduate engineering curricula, this book assumes basic programming skills in a procedural language, such as Java, C#, or C. The examples in the main text should be easy to understand with the help of an introductory book on Java or one of the many online tutorials. Experience shows, however, that difficulties with some basic Java concepts pertain and often cause complications, even at higher levels. The following sections address some of these typical problem spots.

F.1 Arithmetic

Java is a “strongly typed” programming language, which means in particular that any variable has a fixed type that cannot be altered dynamically. Also, the result of an expression is determined by the types of the involved operands and *not* (in the case of an assignment) by the type of the “receiving” variable.

F.1.1 Integer Division

Division involving integer operands is a frequent cause of errors. If the variables **a** and **b** are both of type `int`, then the expression `a / b` is evaluated according to the rules of integer division. The result—the number of times **b** is contained in **a**—is again of type `int`. For example, after the Java statements

```
int a = 2;
int b = 5;
double c = a / b; // resulting value of c is zero!
```

the value of `c` is *not* 0.4 but 0.0 because the expression `a / b` on the right yields the `int`-value 0, which is then automatically converted to the `double` value 0.0.

If we wanted to evaluate `a / b` as a *floating-point* operation (as most pocket calculators do), at least one of the involved operands

must be converted to a floating-point value, such as by an explicit type cast, for example,

```
double c = (double) a / b;    // value of c is 0.4
```

or alternatively

```
double c = a / (double) b;    // value of c is 0.4
```

Example

Assume, for example, that we want to scale any pixel value a of an image such that the maximum pixel value a_{\max} is mapped to 255 (see Ch. 4). In mathematical notation, the scaling of the pixel values is simply expressed as

$$c \leftarrow \frac{a_i}{a_{\max}} \cdot 255$$

and it may be tempting to convert this 1:1 into Java code, such as

```
int a_max = ip.getMaxValue();
for ... {
    int a = ip.getPixel(u,v);
    int c = (a / a_max) * 255; // ← problem!
    ip.putPixel(u, v, c);
}
...
```

As we can easily predict, the resulting image will be all black (zero values), except those pixels whose value was `a_max` originally (they are set to 255). The reason is again that the division `a / a_max` has two operands of type `int`, and the result is thus zero whenever the denominator (`a_max`) is greater than the numerator (`a`).

Of course, the entire operation could be performed in the floating-point domain by converting one of the operands (as we have shown), but this is not even necessary in this case. Instead, we may simply swap the order of operations and start with the multiplication:

```
int c = a * 255 / a_max;
```

Why does this work now? The subexpression `a * 255` is evaluated first,¹ generating large intermediate values that pose no problem for the subsequent (integer) division. Nevertheless, *rounding* should always be considered to obtain more accurate results when computing fractions of integers (see Sec. F.1.5).

F.1.2 Modulus Operator

The result of the modulus operator $a \bmod b$ (used in several places in the main text) is defined [92, p. 82] as the remainder of the “floored” division a/b ,

$$a \bmod b \equiv \begin{cases} a & \text{for } b = 0, \\ a - b \cdot \lfloor a/b \rfloor & \text{otherwise,} \end{cases} \quad (\text{F.1})$$

¹ In Java, expressions at the same level are always evaluated in left-to-right order, and therefore no parentheses are required in this example (though they would do no harm either).

for $a, b \in \mathbb{R}$. This type of operator or library method was not available in the standard Java API until recently.² The following Java method implements the mod operation according to the definition in Eqn. (F.1):³

```
int Mod(int a, int b) {
    if (b == 0)
        return a;
    if (a * b >= 0)
        return a - b * (a / b);
    else
        return a - b * (a / b - 1);
}
```

Note that the *remainder* operator %, defined as

$$a \% b \equiv a - b \cdot \text{truncate}(a/b), \quad \text{for } b \neq 0, \quad (\text{F.2})$$

is often used in this context, but yields the same results only for *positive* operands $a \geq 0$ and $b > 0$. For example,

$$\begin{array}{rcl} 13 \bmod 4 & = & 1 \\ 13 \bmod -4 & = & -3 \\ -13 \bmod 4 & = & 3 \\ -13 \bmod -4 & = & -1 \end{array} \quad \text{vs.} \quad \begin{array}{rcl} 13 \% 4 & = & 1 \\ 13 \% -4 & = & 1 \\ -13 \% 4 & = & -1 \\ -13 \% -4 & = & -1 \end{array}$$

F.1.3 Unsigned Byte Data

Most grayscale and indexed images in Java and ImageJ are composed of pixels of type `byte`, and the same holds for the individual components of most color images. A single byte consists of eight bits and can thus represent $2^8 = 256$ different bit patterns or values, usually mapped to the numeric range $0, \dots, 255$. Unfortunately, Java (unlike C and C++) does *not* provide a suitable “unsigned” 8-bit data type. The primitive Java type `byte` is “signed”, using one of its eight bits for the \pm sign, and is intended to hold values in the range $-128, \dots, +127$.

Java’s `byte` data can still be used to represent the values 0 to 255, but conversions must take place to perform proper arithmetic computations. For example, after execution of the statements

```
int a = 200;
byte b = (byte) p;
```

the variables `a` (32-bit `int`) and `b` (8-bit `byte`) contain the binary patterns

```
a = 000000000000000000000000011001000
b =                               11001000
```

Interpreted as a (signed) `byte` value, with the leftmost bit⁴ as the sign bit, the variable `b` has the decimal value -56 . Thus after the statement

² Starting with Java version 1.8 the mod operation (as defined in Eqn. (F.1)) is implemented by the standard method `Math.floorMod(a, b)`.

³ The definition in Eqn. (F.1) is not restricted to integer operands.

⁴ Java uses the standard “2s-complement” representation, where a sign bit = 1 stands for a negative value.

```
int a1 = b; // a1 == -56
```

the value of the new `int` variable `a1` is -56 ! To (ab-)use signed `byte` data as *unsigned* data, we can circumvent Java's standard conversion mechanism by disguising the content of `b` as a logic (i.e., nonarithmetic) *bit pattern*; for example, by

```
int a2 = (0xff & b); // a2 == 200
```

where `0xff` (in hexadecimal notation) is an `int` value with the binary bit pattern `00000000000000000000000011111111` and `&` is the bitwise AND operator. Now the variable `a2` contains the right integer value (200) and we thus have a way to use Java's (signed) `byte` data type for storing *unsigned* values. Within ImageJ, access to pixel data is routinely implemented in this way, which is considerably faster than using the convenience methods `getPixel()` and `putPixel()`.

F.1.4 Mathematical Functions in Class Math

Java provides most standard mathematical functions as static methods in class `Math`, as listed in Table F.1. The `Math` class is part of the `java.lang` package and thus requires no explicit import to be used. Most `Math` methods accept arguments of type `double` and also return values of type `double`. As a simple example, a typical use of the cosine function $y = \cos(x)$ is

```
double x;
double y = Math.cos(x);
```

Similarly, the `Math` class defines some common numerical constants as static variables; for example, the value of π could be obtained by

```
double pi = Math.PI;
```

Table F.1
 Mathematical methods and constants defined by Java's `Math` class.

<code>double abs(double a)</code>	<code>double max(double a, double b)</code>
<code>int abs(int a)</code>	<code>float max(float a, float b)</code>
<code>float abs(float a)</code>	<code>int max(int a, int b)</code>
<code>long abs(long a)</code>	<code>long max(long a, long b)</code>
<code>double ceil(double a)</code>	<code>double min(double a, double b)</code>
<code>double floor(double a)</code>	<code>float min(float a, float b)</code>
<code>int floorMod(int a, int b)</code>	<code>int min(int a, int b)</code>
<code>long floorMod(long a, long b)</code>	<code>long min(long a, long b)</code>
<code>double rint(double a)</code>	<code>double random()</code>
<code>long round(double a)</code>	
<code>int round(float a)</code>	
<code>double toDegrees(double rad)</code>	<code>double toRadians(double deg)</code>
<code>double sin(double a)</code>	<code>double asin(double a)</code>
<code>double cos(double a)</code>	<code>double acos(double a)</code>
<code>double tan(double a)</code>	<code>double atan(double a)</code>
<code>double atan2(double y, double x)</code>	
<code>double log(double a)</code>	<code>double exp(double a)</code>
<code>double sqrt(double a)</code>	<code>double pow(double a, double b)</code>
<code>double E</code>	<code>double PI</code>

Java's `Math` class (confusingly) offers three different methods for rounding floating-point values:

```
double rint(double x)
long   round(double x)
int    round(float x)
```

For example, a `double` value `x` can be rounded to `int` in any of the following ways:

```
double x; int k;
k = (int) Math.rint(x);
k = (int) Math.round(x);
k = Math.round((float) x);
```

If the operand `x` is known to be positive (as is typically the case with pixel values) rounding can be accomplished without using any method calls by

```
k = (int) (x + 0.5); // only if x >= 0
```

In this case, the expression `(x + 0.5)` is first computed as a floating-point (`double`) value, which is then truncated (toward zero) by the explicit `(int)` typecast.

F.1.6 Inverse Tangent Function

The inverse tangent function $\varphi = \tan^{-1}(a)$ or $\varphi = \arctan(a)$ is used in several places in the main text. This function is implemented by the method `atan(double a)` in Java's `Math` class (Table F.1). The return value of `atan()` is in the range $[-\frac{\pi}{2}, \dots, \frac{\pi}{2}]$ and thus restricted to only two of the four quadrants. Without any additional constraints, the resulting angle is ambiguous. In many practical situations, however, a is given as the ratio of two catheti ($\Delta x, \Delta y$) of a right-angled triangle in the form

$$\varphi = \arctan\left(\frac{y}{x}\right), \quad (\text{F.3})$$

for which we introduced the two-parameter function

$$\varphi = \text{ArcTan}(x, y) \quad (\text{F.4})$$

in the main text. The function `ArcTan(x, y)` is implemented by the standard method `atan2(dy, dx)` in Java's `Math` class (note the reversed parameters though) and returns an unambiguous angle φ in the range $[-\pi, \dots, \pi]$; that is, in any of the four quadrants of the unit circle.⁵ Also, the `atan2()` method returns a useful value even if both arguments are zero.

⁵ The function `atan2(dy, dx)` is available in most current programming languages, including Java, C, and C++.

F.1.7 Classes Float and Double

The representation of floating-point numbers in Java follows the IEEE standard, and thus the types `float` and `double` include the values

<code>Float.MIN_VALUE,</code>	<code>Double.MIN_VALUE,</code>
<code>Float.MAX_VALUE,</code>	<code>Double.MAX_VALUE,</code>
<code>Float.POSITIVE_INFINITY,</code>	<code>Double.POSITIVE_INFINITY,</code>
<code>Float.NEGATIVE_INFINITY,</code>	<code>Double.NEGATIVE_INFINITY,</code>
<code>Float.NaN,</code>	<code>Double.NaN.</code>

These values are defined as constants in the corresponding wrapper classes `Float` and `Double`, respectively. If any `INFINITY` or `NaN`⁶ value occurs in the course of a computation (e.g., as the result of dividing by zero),⁷ Java continues without raising an error, so incorrect values may ripple through a whole chain of calculations, making the actual bugs difficult to locate.

F.1.8 Testing Floating-Point Values Against Zero

Comparing floating-point values or testing them for zero is a non-trivial issue and a frequent cause of errors. In particular, one should *never* write

```
if (x == 0.0) {...} ← problem!
```

if `x` is a floating-point variable. This is often needed, for example, to make sure that it is safe to divide another quantity by `x`. The aforementioned test, however, is not sufficient since `x` may be non-zero but still too small as a divisor.

A much better alternative is to test if `x` is “close” to zero, that is, within some small positive/negative (*epsilon*) interval. While the proper choice of this interval depends on the specific situation, the following settings are usually sufficient for safe operation:⁸

```
static final float EPSILON_FLOAT = 1e-7f;
static final double EPSILON_DOUBLE = 2e-16;

float x;
double y;

if (Math.abs(x) < EPSILON_FLOAT) {
    ... // x is practically zero
}

if (Math.abs(y) < EPSILON_DOUBLE) {
    ... // y is practically zero
}
```

⁶ NaN stands for “not a number”.

⁷ In Java, this only holds for floating-point operations, whereas integer division by zero always causes an *exception*.

⁸ These settings account for the limited *machine accuracy* (ϵ_m) of the IEEE 754 standard types `float` ($\epsilon_m \approx 1.19 \cdot 10^{-7}$) and `double` ($\epsilon_m \approx 2.22 \cdot 10^{-16}$) [190, Ch. 1, Sec. 1.1.2].

F.2.1 Creating Arrays

Unlike in most traditional programming languages (such as FORTRAN or C), arrays in Java can be created *dynamically*, meaning that the size of an array can be specified at runtime using the value of some variable or arithmetic expression. For example:

```
int N = 20;
int[] A = new int[N];
int[] B = new int[N * N];
```

Once allocated, however, the size of any Java array is fixed and cannot be subsequently altered.⁹ Note that Java arrays may be of length *zero*!

After its definition, an array variable can be assigned any other compatible array or the constant value `null`, for example,¹⁰

```
A = B;    // A now references the data in B
B = null;
```

With the assignment `A = B`, the array initially referenced by `A` becomes inaccessible and thus turns into *garbage*. In contrast to C and C++, where unnecessary storage needs to be *deallocated* explicitly, this is taken care of in Java by its built-in “garbage collector”. It is also convenient that newly created arrays of numerical element types (`int`, `float`, `double`, etc.) are automatically initialized to zero.

F.2.2 Array Size

Since an array may be created dynamically, it is important that its actual size can be determined at runtime. This is done by accessing the `length` attribute¹¹

```
int k = A.length; // number of elements in A
```

The size is a property of the array itself and can therefore be obtained inside any method from array arguments passed to it. Thus (unlike in C, for example) it is not necessary to pass the size of an array as a separate function argument.

If an array has more than one dimension, the size (`length`) along every dimension must be queried separately (see Sec. F.2.4). Also arrays are not necessarily rectangular; for example, the rows of a 2D array may have different lengths (including zero).

F.2.3 Accessing Array Elements

In Java, the index of the first array element is always 0 and the index of the last element is $N - 1$ for an array with a total of N elements. To iterate through a 1D array `A` of arbitrary size, one would typically use a construct like

⁹ For additional flexibility, Java provides a number of universal container classes (e.g., the classes `Set` and `List`) for a wide range of applications.

¹⁰ This is not possible if the array variable was defined with the `final` attribute.

¹¹ Notice that the `length` attribute of an array is not a method!

```
for (int i = 0; i < A.length; i++) {  
    // do something with A[i]  
}
```

Alternatively, if only the array *values* are relevant and the array *index* (*i*) is not needed, one could use the following (even simpler) loop construct:

```
for (int a : A) {  
    // do something with array values a  
}
```

In both cases, the Java compiler can generate very efficient runtime code, since the source code makes obvious that the `for` loop does not access any elements outside the array limits and thus no explicit boundary checking is needed at execution time. This fact is very important for implementing efficient image processing programs in Java.

Images in Java and ImageJ are usually stored as 1D arrays (accessible through the `ImageProcessor` method `getPixels()` in `ImageJ`), with pixels arranged in row-first order.¹² Statistical calculations and most point operations can thus be efficiently implemented by directly accessing the underlying 1D array. For example, the `run` method of the contrast enhancement plugin in `Prog. 4.1` (see Chapter 4, p. 58) could also be implemented in the following manner:

```
public void run(ImageProcessor ip) {  
    // ip is assumed to be of type ByteProcessor  
    byte[] pixels = (byte[]) ip.getPixels();  
    for (int i = 0; i < pixels.length; i++) {  
        int a = 0xFF & pixels[i];           // direct read operation  
        int b = (int) (a * 1.5 + 0.5);  
        if (b > 255)  
            b = 255;  
        pixels[i] = (byte) (0xFF & b);     // direct write operation  
    }  
}
```

F.2.4 2D Arrays

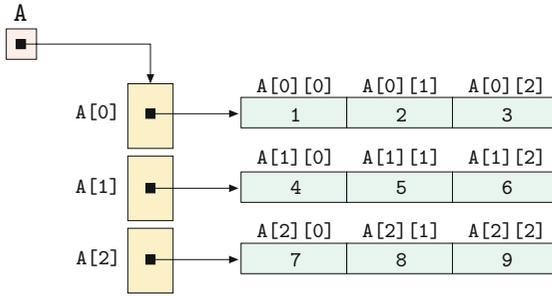
Multidimensional arrays are a frequent source of confusion. In Java, all arrays are 1D in principle, and multi-dimensional arrays are implemented as 1D arrays of arrays etc. (see [Fig. F.1](#)). If, for example, the 3×3 matrix

$$A = \begin{bmatrix} a_{0,0} & a_{0,1} & a_{0,2} \\ a_{1,0} & a_{1,1} & a_{1,2} \\ a_{2,0} & a_{2,1} & a_{2,2} \end{bmatrix} = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix} \quad (\text{F.5})$$

is defined as a 2D `int` array,

```
int [][] A = {{1,2,3},  
              {4,5,6},  
              {7,8,9}};
```

¹² This means that horizontally adjacent image pixels are stored next to each other in computer memory.


Fig. F.1

Layout of elements of a 2D Java array (corresponding to Eqn. (F.5)). In Java, multidimensional arrays are generally implemented as *1D* arrays whose elements are again *1D* arrays.

then A is actually a *1D* array with three elements, each of which is again a *1D* array. The elements $A[0]$, $A[1]$ and $A[2]$ are of type `int[]` and correspond to the three rows of the matrix A (see Fig. F.1).

The usual assumption is that the array elements are arranged in *row-first* order, as illustrated in Fig. F.1. The first index thus corresponds to the *row* number r and the second index corresponds to the *column* number c , that is,

$$a_{r,c} \equiv A[r][c]. \quad (\text{F.6})$$

This conforms to the mathematical convention and makes the array definition in the code segment above look exactly the same as the original matrix in Eqn. (F.5). Note that in this scheme the first array index corresponds to the *vertical* coordinate and the second index to the *horizontal* coordinate.

However, if an array is used to specify the contents of an *image* $I(u, v)$ or a *filter kernel* $H(i, j)$, we usually assume that the first index (u or i , respectively) is associated with the horizontal x -coordinate and the second index (v bzw. j) with the vertical y -coordinate. For example, if we represent the filter kernel

$$H = \begin{bmatrix} h_{0,0} & h_{1,0} & h_{2,0} \\ h_{0,1} & h_{1,1} & h_{2,1} \\ h_{0,2} & h_{1,2} & h_{2,2} \end{bmatrix} = \begin{bmatrix} -1 & -2 & 0 \\ -2 & 0 & 2 \\ 0 & 2 & 1 \end{bmatrix}$$

as a 2D Java array,

```
double[][] H = {{-1,-2, 0},
                {-2, 0, 2},
                { 0, 2, 1}};
```

then the row and column indexes must be *reversed* in order to access the correct elements. In this case we have the relation

$$h_{i,j} \equiv H[j][i], \quad (\text{F.7})$$

that is, the ordering of the indexes for array H is not the same as for the i/j coordinates of the filter kernel. In this case the *first* array index (j) corresponds to the *vertical* coordinate and the *second* index (i) to the *horizontal* coordinate. The advantage is that (as shown in the aforementioned code segment) the definition of the filter kernel

can be written in the usual matrix form¹³ (otherwise we would have to specify the transposed kernel matrix).

If a 2D array is merely used as an image container (whose contents are never defined in matrix form) any convention can be used for the ordering of the indexes. For example, the ImageJ method `getFloatArray()` of class `ImageProcessor`, when called in the form

```
float[][] I = ip.getFloatArray();
```

returns the image as a 2D array (`I`), whose indexes are arranged in the usual x/y order, that is,

$$I(x, y) \equiv I[x][y]. \quad (\text{F.8})$$

In this case, the image pixels are arranged in column-order, that is, *vertically* adjacent elements are stored next to each other in memory.

Size of multi-dimensional arrays

The size of a multi-dimensional array can be obtained by querying the size of its sub-arrays. For example, given the following 3D array with dimensions $P \times Q \times R$,

```
int A[][][] = new int[P][Q][R];
```

the size of `A` along its three dimensions is obtained by the statements

```
int p = A.length;           // = P
int q = A[0].length;        // = Q
int r = A[0][0].length;     // = R
```

This at least works for “rectangular” Java arrays, that is, multi-dimensional arrays with all sub-arrays at the same level having *identical* lengths, which is warranted by the array initialization in the aforementioned case. However, every 1D sub-array of `A` may be replaced by a suitable 1D array of *different* length,¹⁴ for example, by the statement

```
A[0][0] = new int[0];
```

To avoid “index-out-of-bounds” errors, the length of each sub-array should be determined dynamically. The following example shows a “bullet-proof” iteration over all elements of a 3D array `A` whose sub-arrays may have different lengths or may even be empty:

```
int A[][][];
...
for (int i = 0; i < A.length; i++) {
    for (int j = 0; j < A[i].length; j++) {
        for (int k = 0; k < A[i][j].length; k++) {
            // safely access A[i][j][k]
        }
    }
}
```

¹³ This scheme is used, for example, in the implementation of the 3×3 filter plugin in Prog. 5.2 (Chapter 5, p. 95).

¹⁴ Even if the array `A` was originally declared `final`, the structure and contents of its sub-arrays may be modified any time.

In Java, as mentioned earlier, we can create arrays dynamically; that is, the size of an array can be specified at runtime. This is convenient because we can adapt the size of the arrays to the given problem. For example, we could write

```
Corner[] corners = new Corner[n];
```

to create an array that can hold `n` objects of type `Corner` (as defined in Chapter 7, Sec. 7.3). Note that the new array `corners` is not filled with corners yet but initialized with `null` references, so the newly created array holds no objects at all. We can insert a `Corner` object into its first (or any other) cell, for example, by

```
corners[0] = new Corner(10, 20, 6789.0f);
```

F.2.6 Searching for Minimum and Maximum Values

Unfortunately, the standard Java API does not provide methods for retrieving the minimum and maximum values of a numeric array. Although these values are easily found by iterating over all elements of the sequence, care must be taken regarding the initialization.

For example, finding the extreme values of a sequence of `int`-values could be accomplished as follows:¹⁵

```
int[] A = ...
int minval = Integer.MAX_VALUE;
int maxval = Integer.MIN_VALUE;
for (int val : A) {
    minval = Math.min(minval, val);
    maxval = Math.max(maxval, val);
}
```

Note the use of the constants `MIN_VALUE` and `MAX_VALUE`, which are defined for any numeric Java type.

However, in the case of *floating-point* values, these are not the proper values for initialization.¹⁶ Instead, `POSITIVE_INFINITY` and `NEGATIVE_INFINITY` should be used, as shown in the following code segment:

```
double[] B = ...
double minval = Double.POSITIVE_INFINITY;
double maxval = Double.NEGATIVE_INFINITY;
for (double val : B) {
    minval = Math.min(minval, val);
    maxval = Math.max(maxval, val);
}
```

¹⁵ Alternatively, one could initialize `minval` and `maxval` with the first array element `A[0]`.

¹⁶ Because `Double.MIN_VALUE` and `Float.MIN_VALUE` specify to the smallest *positive* values.

F.2.7 Sorting Arrays

Arrays can be sorted efficiently with the standard method

```
Arrays.sort(type[] arr)
```

in class `java.util.Arrays`, where `arr` can be any array of primitive *type* (`int`, `float`, etc.) or an array of objects. In the latter case, the array may not have `null` entries. Also, the class of every contained object must implement the `Comparable` interface, that is, provide a public method `compareTo()` that returns an `int` value of `-1`, `0`, or `1`, depending upon the intended ordering relation. For example, the class `Corner` defines the `compareTo()` method as follows:

```
public class Corner implements Comparable<Corner> {
    float x, y, q;
    ...
    public int compareTo(Corner other) {
        if (this.q > other.q) return -1;
        else if (this.q < other.q) return 1;
        else return 0;
    }
}
```

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