Appendix A
Basics on Graph Theory

We review in this chapter the most elementary notions of graph theory and present in passing a few graph-theoretical theorems of combinatorial nature that have actually played a role in other chapters. Throughout the book we have tacitly adopted all notations presented in this Appendix.

Definition A.1. A *directed graph*, or *digraph*, is a pair $G = (V, E)$, where V is a (finite or countable) set and E is a subset of $V \times V$. We refer to the elements of V and E as *nodes* and *edges*, respectively. A digraph is said to be *simple* if for any two elements $v, w \in V$

(S1) at most one of the pairs $e := (v, w), \bar{e} := (w, v)$ is an element of E and
(S2) the pair (v, v) is not an element of E.

Simple digraph are called *oriented graphs*. We call G *finite* if so are V and hence E. The *initial* and *terminal endpoint* (or sometimes: *tail* and *head*) of $e \equiv (v, w)$ are v and w, respectively. We denote them by

$$e_{\text{init}} := v \quad \text{and} \quad e_{\text{term}} := w, \tag{A.1}$$

and say that they are *adjacent* (shortly: $v \sim w$) and more precisely that v *precedes* w, or that w *follows* v; or that they are *neighbors*. One also says that e is *incident* in v (as well as in w); and that two edges are adjacent if they share and endpoint.

(Observe that this notion of edge adjacency is independent of orientation.)

Conditions (S1) and (S2) stipulate that there are no multiple edges between two nodes, and no loops connecting one node to itself.

Definition A.2. A *simple graph* is an oriented graph the orientations of whose edges are ignored; i.e., any edge is a set of the form $\{v, w\}$ for $v, w \in V$ with $v \neq w$.

Conversely, an oriented graph *over* a given simple graph is determined fixing the orientation of each of its edges—clearly, there are $2^{|E|}$ different oriented graphs over the same simple graph. One can show by a simple double counting argument that for all simple graphs the *Handshaking Lemma*

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$$|\mathsf{E}| = \frac{1}{2}\sum_{\mathsf{v}\in\mathsf{V}} \deg(\mathsf{v}) \tag{A.2}$$

holds.

Definition A.3. Let $\mathsf{G} = (\mathsf{V}, \mathsf{E})$ be an oriented graph.

1. A *subgraph* of G is an oriented graph $\tilde{\mathsf{G}} = (\tilde{\mathsf{V}}, \tilde{\mathsf{E}})$ such that $\tilde{\mathsf{V}} \subset \mathsf{V}$ and $\tilde{\mathsf{E}} \subset \mathsf{E}$. The subgraph is called *induced* if additionally
$$\mathsf{v}, \mathsf{w} \in \tilde{\mathsf{V}} \text{ and } (\mathsf{v}, \mathsf{w}) \in \mathsf{E} \qquad \text{implies} \qquad (\mathsf{v}, \mathsf{w}) \in \tilde{\mathsf{E}}.$$
2. If any two nodes are adjacent, then G is called *complete*.
3. Nodes with no neighbors are said to be *isolated*. Nodes with only one neighbor are called *leaves*. A node is *inessential* if it has exactly two neighbors. *Ramification nodes* are those with at least three neighbors.
4. If $\mathsf{v}, \mathsf{w} \in \mathsf{V}$ and $n \in \mathbb{N}$, then an *n-path* from v to w is a pair of sequences
$$(\mathsf{v}_1, \dots, \mathsf{v}_{n+1}) \in \mathsf{V}^{n+1} \qquad \text{and} \qquad (\mathsf{e}_1, \dots, \mathsf{e}_n) \in \mathsf{E}^n,$$
where $\mathsf{v}_1 = \mathsf{v}$, $\mathsf{v}_{n+1} = \mathsf{w}$, and for all $i = 1, \dots, n$ either $\mathsf{e}_i = (\mathsf{v}_i, \mathsf{v}_{i+1})$ or $\mathsf{e}_i = (\mathsf{v}_{i+1}, \mathsf{v}_i)$. A path from v to w is called *closed* if $\mathsf{v} = \mathsf{w}$; it is called *oriented* if $\mathsf{e}_i = (\mathsf{v}_i, \mathsf{v}_{i+1})$ for all $i = 1, \dots, n$. A path all of whose edges are distinct is called a *trail*.
5. One defines an equivalence relation identifying all closed paths that consist of sequences of nodes and edges that are equal up to some shift. The representative of a corresponding equivalence class is called a *circuit*, or sometimes a *periodic orbit*. A circuit is uniquely determined by the sequence of its edges.
6. Because a circuit is allowed to contain the same nodes and even the same edges, one can produce a new circuit $\mathsf{C} = n \cdot \mathsf{C}_0$ out of an old one C_0 by repeating n times all its nodes and edges in the same sequence. Given a circuit C, its *gene* (or sometimes: *primitive*) $\mathrm{Gen}(\mathsf{C})$ is the circuit such that $\mathsf{C} = n \cdot \mathrm{Gen}(\mathsf{C})$ for the largest possible $n \in \mathbb{N}$.
7. A *cycle* is a closed path whose nodes (with the exception of the initial and terminal one) and edges are pairwise different. An *oriented cycle* is an oriented path that is a cycle.
8. If for any two nodes $\mathsf{v}, \mathsf{w} \in \mathsf{V}$ there is a path from v to w, then G is called *connected*, and *strongly connected* if the path can be chosen to be oriented. A *connected/strongly connected component* of G is a largest connected/strongly connected subgraph.
9. A subgraph of G is called a *forest* if none of its subgraphs is a cycle as subgraph, and a *tree* if additionally it is connected. It is called a *spanning tree* of G if its node set agrees with V. One checks that G is a forest if and only if
$$|\mathsf{E}| - |\mathsf{V}| + \kappa = 0, \tag{A.3}$$

where κ is the number of connected components. Indeed, $|\mathsf{E}| - |\mathsf{V}| + \kappa$ is the number of independent cycles contained in G, cf. [15, § 5], and is thus called *cyclomatic number* (or sometimes *first Betti number*) of G.

10. If there is one node $\mathsf{v} \in \mathsf{V}$—which is then called *center*—such that any further $\mathsf{w} \in \mathsf{V}$ is adjacent to v, and only to it, then G is a *star*. If the center is initial/terminal endpoint of each edge, then G is called *outbound*/*inbound star*, respectively; in either case it is an *oriented star*.
11. If V can be partitioned in two subsets $\mathsf{V}_1, \mathsf{V}_2$ such that $(\mathsf{v}, \mathsf{w}) \not\in \mathsf{E}$ for any two nodes $\mathsf{v}, \mathsf{w} \in \mathsf{V}_i$, $i = 1, 2$, then G is called *bipartite*. If furthermore each node v in V_1 and each node in V_2 is initial and terminal endpoint of any incident edge, respectively, then G is called *orientedly bipartite*.
12. An *Eulerian tour* of G is a closed trail C in G whose edge set $\tilde{\mathsf{E}}$ agrees with E. If G contains an Eulerian tour C, then G is called *Eulerian*. If its orientation makes C an *oriented* cycle, then we call G *orientedly Eulerian*.

Example A.4. $(\mathsf{v}, \mathsf{w}, \mathsf{z}, \mathsf{v})$, $((\mathsf{v}, \mathsf{w}), (\mathsf{w}, \mathsf{z}), (\mathsf{z}, \mathsf{v}))$ on the one hand, and $(\mathsf{w}, \mathsf{z}, \mathsf{v}, \mathsf{w})$ and $((\mathsf{w}, \mathsf{z}), (\mathsf{z}, \mathsf{v}), (\mathsf{z}, \mathsf{w}))$ on the other hand, are two representatives of the same circuit.

Remarks A.5. 1) We do not regard paths as subgraphs of G, since they may in general contain the same nodes and even the same edges more than once; but suitably identifying all such paths yields one representative that is indeed an induced subgraph of G. (Loosely speaking, this is the "union" of all the nodes and edges that belong to the given path.)

2) A cycle can be equivalently defined as a connected graph each of whose nodes has exactly two neighbors.
3) A graph is a closed trail if and only if it is a circuit that agrees with its gene. Each closed trail C in G, and in particular each cycle, can thus be identified with one vector $z \in \mathbb{C}^{\mathsf{E}}$ defined by

$$z(\mathsf{e}) := \begin{cases} 1 \text{ if } \mathsf{e} \text{ belongs to the edge set of } \mathsf{C}, \\ 0 \text{ otherwise.} \end{cases}$$

4) Non-oriented Eulerian graphs can be given an orientation in a natural way. With respect to this orientation, they are also strongly connected.

If we consider two *triangle graphs*, i.e., two simple graphs consisting of three nodes and three edges each, then as soon as one draws them one sees that they can be identified. We can formalize this intuition as follows.

Definition A.6. Let $\mathsf{G} = (\mathsf{V}, \mathsf{E}), \tilde{\mathsf{G}} = (\tilde{\mathsf{V}}, \tilde{\mathsf{E}})$ be oriented graphs.

A bijective mapping $O : \mathsf{V} \to \tilde{\mathsf{V}}$ is called an *isomorphism* whenever for all $\mathsf{v}, \mathsf{w} \in \mathsf{V}$ $(O\mathsf{v}, O\mathsf{w}) \in \tilde{\mathsf{E}}$ or $(O\mathsf{w}, O\mathsf{v}) \in \tilde{\mathsf{E}}$ if and only if $(\mathsf{v}, \mathsf{w}) \in \mathsf{E}$ or $(\mathsf{w}, \mathsf{v}) \in \mathsf{E}$; and a *automorphism* if $\mathsf{G} = \tilde{\mathsf{G}}$. The set of all automorphisms of G forms the *automorphism group* of G, which we denote by $\mathrm{Aut}(\mathsf{G})$.

Fig. A.1 The Petersen graph

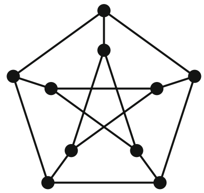
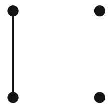


Fig. A.2 A graph for which Aut(G) and Aut′(G) are not isomorphic



A bijective mapping $U : \mathsf{E} \to \tilde{\mathsf{E}}$ is called an *edge isomorphism* whenever for all $\mathsf{e}, \mathsf{f} \in \mathsf{E}$ $U(\mathsf{e}), U(\mathsf{f})$ are adjacent (in the sense of Definition A.1) if and only if e, f are adjacent; and an *edge automorphism* if $\mathsf{G} = \tilde{\mathsf{G}}$. The set of all edge automorphisms of G forms the *edge automorphism group* of G, which we denote by $\mathrm{Aut}^*(\mathsf{G})$.

Observe that all nodes that belong to the same orbit induced by some subgroup of the automorphism group of a graph have necessarily the same number of neighbors.

Example A.7. The Petersen graph in Fig. A.1 is probably the single most famous finite graph. The automorphism group of this graph is isomorphic to the symmetric group S_5. It acts on the graph's nodes by arbitrary permutations of the outer nodes: this determines uniquely the action on the inner nodes, too.

In other words, automorphisms (resp., edge automorphisms) are node (resp., edge) permutations that preserve node (resp., edge) adjacency. Corresponding notions hold if $\mathsf{G}, \tilde{\mathsf{G}}$ are simple graphs, as the above notion does not depend on orientation.

Now, observe that each symmetry $O \in \mathrm{Aut}(\mathsf{G})$ naturally induces an edge symmetry $U := \tilde{O} \in \mathrm{Aut}^*(G)$: simply define

$$\tilde{O}(e) := (O\mathsf{v}, O\mathsf{w}) \qquad \text{whenever } \mathsf{e} = (\mathsf{v}, \mathsf{w}).$$

While clearly

$$\mathrm{Aut}'(\mathsf{G}) := \{\tilde{O} : O \in \mathrm{Aut}(\mathsf{G})\}$$

(whose elements we call *induced edge automorphisms*) is a group, it can be strictly smaller than $\mathrm{Aut}(\mathsf{G})$—simply think of the graph G defined in Fig. A.2. There, $\mathrm{Aut}(\mathsf{G}) = C_2 \times C_2$ (independent switching of the adjacent nodes and/or of the isolated nodes) but $\mathrm{Aut}'(\mathsf{G})$ is trivial, so $\mathrm{Aut}(\mathsf{G})$ and $\mathrm{Aut}'(\mathsf{G})$ are not isomorphic.

However, this is an exceptional case. The following has been proved by G. Sabidussi and H. Whitney, cf. [13, Thm. 1] and [2, Cor. 9.5b].

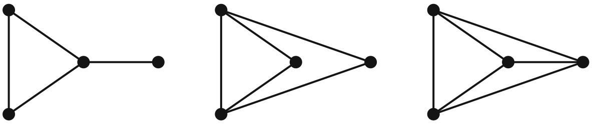


Fig. A.3 The only graphs on four or more nodes for which Aut(G), Aut*(G) are not isomorphic

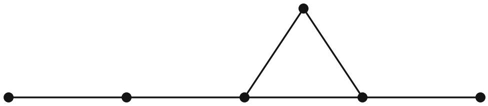


Fig. A.4 A graph without any non-trivial automorphisms

Lemma A.8. *Let* G *be an (either oriented or simple) finite graph. Then the groups* Aut(G) *and* Aut′(G) *are isomorphic provided that* G *contains at most one isolated node and no isolated edge.*

If additionally G *is connected and has at least three nodes, then the three groups* Aut(G), Aut′(G), Aut*(G) *are pairwise isomorphic if and only if G is different from each of the graphs in Fig. A.3.*

The following *Frucht's theorem* is one of the most interesting result in the theory of graph automorphisms. It was proved in [9] and strengthened in [14, 21, 22].

Theorem A.9. *For any group Γ there are uncountably many connected* cubic *graphs* G*—i.e., graphs each of whose nodes has exactly three neighbors—such that* Aut(G) *is isomorphic to Γ.*

If the automorphism group of G is transitive, then G is said to be *node transitive*. A necessary condition for a graph to be node transitive is that each node has the same number of neighbors.

It was observed in [7] that finite graphs can only exceptionally have non-trivial automorphisms: This assertion can be given a precise meaning in the theory of random graphs. An elementary example of a graph with only trivial automorphisms is depicted in Fig. A.4.

L. Euler found in [8] a sufficient and necessary condition for a finite graph to be Eulerian. His result was extended to the infinite case in [6].

Theorem A.10. *Let* $\mathsf{G} = (\mathsf{V}, \mathsf{E})$ *be a connected (non-oriented) graph.*

(1) If G *is finite, then it is Eulerian if and only if each of its nodes has an even number of incident edges; it is orientedly Eulerian if and only if each of its nodes has an equal number of incoming and outgoing edges.*

(2) If G *is infinite, then it is Eulerian if and only if*

- E *is at most countable,*
- *each node has an even or infinite number of neighbors,*
- *if* $\mathsf{E}' \subset \mathsf{E}$ *is finite, then the connected components of* $\mathsf{G}' := (\mathsf{V}, \mathsf{E} \setminus \mathsf{E}')$ *are at most two, and in fact exactly one if each node has an even number of neighbors in* G'.

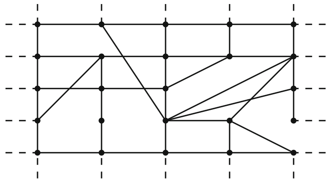


Fig. A.5 A non-regular infinite Eulerian graph

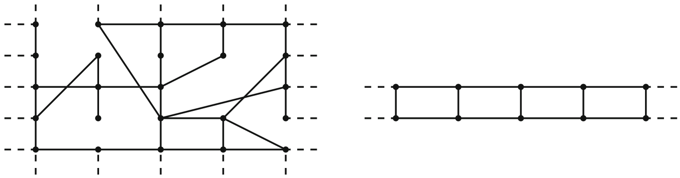


Fig. A.6 Two infinite non-Eulerian graphs

Example A.11. An example of infinite Eulerian graph is given as follows: The *oriented d-dimensional lattice* is the oriented graph (V, E) whose set is $\mathsf{V} = \mathbb{Z}^d$ and whose edge set E is defined as follows: For any two vectors $x, y \in \mathbb{Z}^d$, $(x, y) \in \mathsf{E}$ if and only if there is exactly *one* $k_0 \in \{1, \ldots, d\}$ such that

$$y_{k_0} - x_{k_0} = 1 \qquad \text{and} \qquad y_k = x_k \quad \text{for all } k \neq k_0.$$

I.e., all edges of $\mathbb{Z}^d$ are of the form $(x, x + e_k)$ for some $x \in \mathbb{Z}^d$ and $k = 1, \ldots, d$, where e_k is the k-th vector of the canonical basis of $\mathbb{Z}^d$. Accordingly, each edge is oriented in the direction of the first orthant.

If we discard this orientation, we obtain the *plain d-dimensional lattice*, which by Theorem A.10.(2) is Eulerian if and only if $d > 1$. One can easily modify this setting to obtain non-regular Eulerian graphs, e.g. through a local perturbation like in Fig. A.5.

Definition A.12. The *doubling* of a digraph $\mathsf{G} = (\mathsf{V}, \mathsf{E})$ is the digraph $\mathsf{G}^{\parallel} := (\mathsf{V}, \overline{\mathsf{E}})$, where $\overline{\mathsf{E}} := \{\mathsf{e}, \bar{\mathsf{e}} : \mathsf{e} \in \mathsf{E}\}$.

Hence, the doubling of a digraph is the digraph obtained adding to each oriented edge $\mathsf{e} \in \mathsf{E}$ its reverse $\bar{\mathsf{e}}$. Clearly, $\mathsf{G}^{\parallel}$ is not simple even if G is so (more precisely, (S2) is not satisfied by G).

Remark A.13. The doubling $\mathsf{G}^{\parallel}$ is at most countable and each node has an even or infinite number of neighbors for any digraph G. However, the third condition in Theorem A.10.(2) may well fail for $\mathsf{G}^{\parallel}$, too: think e.g. of the doubling of the infinite path graph $\mathbb{Z}$, and more generally of any infinite tree. Also the right graph in Fig. A.6 has a non-Eulerian doubling. However, this condition is satisfied by the doubling of the planar lattice $\mathbb{Z}^2$, and more generally by any finite perturbation of a graph associated with a tiling of the plane, provided all tiles are bounded: The left graph in Fig. A.6 is not Eulerian, but its doubling is.

Definition A.14. A *weighted digraph* is a triple $\mathsf{G} = (\mathsf{V}, \mathsf{E}, \rho)$, where (V, E) is a digraph and $\rho : \mathsf{E} \to (0, \infty)$ is some given function such that $\rho(\mathsf{e}) = \rho(\bar{\mathsf{e}})$ whenever both $\mathsf{e}, \bar{\mathsf{e}} \in \mathsf{E}$. A *weighted oriented graph* is a weighted, simple digraph.

Weighted oriented graphs with both sinks and sources have been often called *networks* since the 1940s, in particular by the Cambridge school during their investigations on the axiomatic theory of electric circuits, cf. [4] and subsequent papers.

Conventions A.15. *(1) We always regard unweighted graphs as weighted ones upon imposing* $\rho \equiv 1$. *All notions defined for weighted graphs thus extend to unweighted ones. Conversely, all notions that only rely upon a graph's connectivity (e.g., existence of an Eulerian graph) remain unchanged if a weight function is introduced.*

(2) If G *is weighted, we regard its subgraphs as weighted with respect to the function* $\tilde{\rho} := \rho_{|\tilde{\mathsf{E}}}$.

Example A.16. Weights can be used to effectively deform a given graph without affecting its connectivity. E.g., the lattice graph $\mathbb{Z}^d$, cf. Example A.11, can be turned into a weighted oriented graph $(\mathbb{Z}^d, \rho)$ in which each pair (v, w) of adjacent nodes is distant $\rho\big((\mathsf{v}, \mathsf{w})\big)$ length units. If in particular $\rho \equiv \rho_0 > 0$, then ρ_0 is referred to as *lattice constant*. Clearly, modifying ρ_0 leads to a rescaling of the whole lattice. Heuristically, one expects that discretized equations on $\mathbb{Z}^d$ tend to their continuous counterparts in $\mathbb{R}^d$ whenever the lattice constant tends to 0. This is a favorite empirical principle in the treatment of a number of problems in physics, and in particular in the so-called *lattice field theory*.

Definition A.17. Let $\tilde{\mathsf{G}}$ be a subgraph of a weighted oriented graph $\mathsf{G} = (\mathsf{V}, \mathsf{E}, \rho)$. Then *capacity* and *volume* of $\tilde{\mathsf{G}}$ are defined by

$$\mathrm{cap}_\rho(\tilde{\mathsf{G}}) := \prod_{\mathsf{e} \in \tilde{\mathsf{E}}} \rho(\mathsf{e}) \qquad \text{and} \qquad \mathrm{vol}_\rho(\tilde{\mathsf{G}}) := |\tilde{\mathsf{E}}|_\rho \sum_{\mathsf{e} \in \tilde{\mathsf{E}}} \rho(\mathsf{e}),$$

respectively. The *surface of* $\tilde{\mathsf{G}}$ *with respect to a weight function* $\nu : \mathsf{V} \to (0, \infty)$, or simply *surface* if $\nu \equiv 1$, is defined as

$$\mathrm{surf}_\nu(\tilde{\mathsf{G}}) := |\tilde{\mathsf{V}}|_\nu := \sum_{\mathsf{v} \in \tilde{\mathsf{V}}} \nu(\mathsf{v}).$$

Using the notation of Chap. 3, it is clear that a graph has finite surface with respect to ν (resp., finite volume with respect to ρ) if and only if $\nu \in \ell^1(\mathsf{V})$ (resp., if and only if $\rho \in \ell^1(\mathsf{E})$).

Clearly, the surface of $\tilde{\mathsf{G}}$ is simply the cardinality of $\tilde{\mathsf{V}}$ if $\nu \equiv 1$; and by the Handshaking Lemma (cf. (A.2)) $\mathsf{G} = (\mathsf{V}, \mathsf{E}, \rho)$ has finite volume if and only if G has finite surface with respect to $\nu = \deg_\rho$.

Remark A.18. In the specific case of paths or cycles, the word *length* is universally used in the literature instead of *volume*. We also adopt this convention and for a path $\tilde{\mathsf{G}} := \mathsf{P}$ we denote its length by $\text{len}_\rho(\mathsf{P})$. The same notation extends in a natural way to circuits.

Clearly, in the unweighted case surface and volume of a subgraph are simply the cardinalities of its node and edge set, respectively, whereas its capacity is always 1 unless G is empty.

One of the reasons why graphs are so popular in the applied sciences is that it is easy to identify real-life objects with graph-like structures. Conversely, also the following holds.

Lemma A.19. *Each (oriented or simple) graph* $\mathsf{G} = (\mathsf{V}, \mathsf{E})$ *can be embedded in* $\mathbb{R}^3$*, i.e., it is possible*

(1) to associate to each node $\mathsf{v} \in \mathsf{V}$ *a point* $x_\mathsf{v} \in \mathbb{R}^3$ *in an injective way, and*
(2) to connect two points $x_\mathsf{v}, x_\mathsf{w}$ *by an three-dimensional simple arc* s_{vw} *if and only if* v, w *are adjacent, in such a way that different arcs do not share any internal points.*

The embedding can be e.g., performed by associating each $\mathsf{v} \in \mathsf{V}$ with a different point of the x-axis and then connecting each pair (v, w) of adjacent nodes by a simple arc that lies in one of the uncountably many different planes that contain the x-axis, choosing a different plane for each pair.

Accordingly, we may identify edges with simple arcs, although this identification clearly depends on the chosen embedding. This is the first step towards the development of the theory of metric graphs presented in Sect. 3.2.

It is sometimes useful to switch from a description of a system based on agents (persons, particles, nations…) to one based on their interactions: E.g., Feynman diagrams in quantum field theory [24], p-graphs in anthropology [25], or highway networks from our Model 2 in Chap. 1 are based on this idea. The following formalism goes back to [12].

Definition A.20. Let $\mathsf{G} = (\mathsf{V}, \mathsf{E})$ be a simple graph. Its *line graph* is the simple graph $\mathsf{G}_L := (\mathsf{V}_L, \mathsf{E}_L)$ with node set $\mathsf{V}_L := \mathsf{E}$ and such that for any $\mathsf{e}, \mathsf{f} \in \mathsf{V}_L$ $(\mathsf{e}, \mathsf{f}) \in \mathsf{E}_L$ if and only if e, f have a common endpoint.

Definition A.21. Let $\mathsf{G} = (\mathsf{V}, \mathsf{E})$ be an oriented graph. Its *line graph* is the oriented graph $\mathsf{G}_L := (\mathsf{V}_L, \mathsf{E}_L)$ with node set $\mathsf{V}_L := \mathsf{E}$ and such that for any $\mathsf{e}, \mathsf{f} \in \mathsf{V}_L$ $(\mathsf{e}, \mathsf{f}) \in \mathsf{E}_L$ if and only if $\mathsf{e}_{\text{term}} = \mathsf{f}_{\text{init}}$.

If now $\mathsf{G} = (\mathsf{V}, \mathsf{E}, \rho)$ is a *weighted* oriented graph, then its line graph is $\mathsf{G}_L := (\mathsf{V}_L, \mathsf{E}_L, \rho_L)$, where $\mathsf{V}_L, \mathsf{E}_L$ are constructed as before and the weight function ρ_L is defined by $\rho_L((\mathsf{e}, \mathsf{f})) := \rho(\mathsf{f})$.

Comparing Definitions A.20 and A.21 one sees that for two nodes $\mathsf{e}, \mathsf{f} \in \mathsf{V}_L$ the edge (e, f) may belong to the edge set of the *non-oriented* version of the line graph even if neither (e, f) nor (f, e) belong to the edge set of the *oriented* line graph: this is the case precisely when they share either the initial endpoint or the terminal endpoint—i.e., e, f form an oriented star, rather than an oriented path.

Appendix B
Basics on Sobolev Spaces

One of the most fruitful mathematical ideas of the last century is the weak formulation of differential equations. One weakens the notion of solution of a boundary value differential problem, looks for a solution in a suitably larger class (which typically allows one to use standard Hilbert space methods, like the Representation Theorem of Riesz–Fréchet) and eventually proves that the obtained solution is in fact also a solution in a classical sense. The essential idea behind this approach is that of *weak derivative*, one which is based on replacing the usual property of differentiability by a prominent quality of differentiable functions—the possibility to integrate by parts.

Definition B.1. Let $I \subset \mathbb{R}$ be an open interval, whose boundary we denote by ∂I, and $p \in [1, \infty]$. A function $f \in L^p(I)$ is said to be *weakly differentiable* if there exists $g \in L^p(I)$ such that

$$\int_I f h' = -\int_I g h \qquad \text{for all } h \in C_c^\infty(I). \tag{B.1}$$

The function g is unique and is called the *weak derivative* of f, shortly: $g := f'$. The set of weakly differentiable functions $f \in L^p(I)$ such that $f' \in L^p(I)$ is denoted by $W^{1,p}(I)$ and called *Sobolev space of order 1.* We define the Sobolev space $W^{k,p}(I)$ of order $k \geq 2$ recursively as the set of those functions $f \in W^{k-1,p}(I)$ such that $f^{(k-1)}$, the weak derivative of order $k-1$, belongs to $W^{1,p}(I)$.

If $c \in L^\infty(I)$, then $\tilde{g} \in \mathbb{K}^{\partial I}$ is said to be *conormal derivative of f (with respect to c)* if

$$\int_I c f' h' + \int_I (c f')' h = \int_{\partial I} \tilde{g} h_{|\partial I} \qquad \text{for all } h \in W^{1,p}(I). \tag{B.2}$$

In this case, $\tilde{g}$ is unique and is denoted by $\frac{\partial_c f}{\partial \nu}$.

If I is bounded, then by Hölder's inequality $W^{1,p}(I)$ is continuously embedded in $W^{1,q}(I)$ for all $p, q \in [1, \infty]$ such that $p \geq q$.

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Lemma B.2. *Let I be an open interval, $k \in \mathbb{N}$ and $p \in [1, \infty]$. Then $W^{k,p}(I)$ is a Banach space with respect to the norm defined by*

$$\|f\|^p_{W^{k,p}(I)} := \sum_{j=1}^{k} \|f^{(j)}\|^p_{L^p(I)}.$$

It is separable if $p \in [1, \infty)$ and reflexive if $p \in (1, \infty)$.

Furthermore, $W^{k,2}(I)$ is a Hilbert space with respect to the inner product

$$(f|g)_{W^{k,2}(I)} := \sum_{j=1}^{k} (f^{(j)}|g^{(j)})_{L^2(I)} = \sum_{j=1}^{k} \int_0^1 f^{(j)}(x)\overline{g^{(j)}(x)}dx.$$

Furthermore, the space $C^1(\overline{I})$ is densely and continuously embedded in $W^{1,p}(I)$, since any $f \in C^1(\overline{I})$ satisfies (B.1) (which for continuously differentiable functions is nothing but the usual formula of integration by parts) with $g := -f'$.

The following results are special cases of [1, Thm. 4.12], [3, Thm. 8.8, Rem. 8.10, and § 8.1.(iii)] and [10, Satz 1]. We denote by $C_b(\overline{I})$ the space of continuous functions on $\overline{I}$ and by $C_0(\overline{I})$ its closed subspace consisting of those bounded continuous functions on $\overline{I}$ such that for all $\epsilon > 0$ $\{x \in I : |f(x)| \geq \epsilon\}$ is compact. (Clearly, $C_b(\overline{I}) = C_0(I)$ if I is finite; otherwise, it consists of those continuous functions that vanish at ∞.) Lemma B.3.(2) is usually referred to as *Rellich–Kondrachov Theorem*.

Lemma B.3. *Let $I \subset \mathbb{R}$ be an open interval. Then the following assertions hold.*

(1) $W^{1,p}(I) \overset{d}{\hookrightarrow} C_0(I)$, i.e., $W^{1,p}(I)$ is densely and continuously embedded in $C_0(I)$ for all $p \in [1, \infty]$.
(2) If I is bounded, then both the embeddings of $W^{1,1}(I)$ in $L^q(I)$ and of $W^{1,p}(I)$ in $C(\overline{I})$ are compact, for all $p, q < \infty$.
(3) The embedding of $W^{1,2}(I)$ in $L^2(I)$ is a Hilbert–Schmidt operator, provided I is bounded.
(4) $C^\infty(I)$ is dense in $W^{1,p}(I)$.
(5) $C_c^\infty(\mathbb{R})$ is dense in $W^{1,p}(\mathbb{R})$ but $C_c^\infty(I)$ is not dense in $W^{1,p}(I)$ whenever I is bounded.

Remark B.4. In order to explain some notions used in Lemma B.3, let us recall that a linear operator T from H_1 to H_2, where H_1, H_2 are Hilbert spaces, is said to be of *p-th Schatten class* (short: $T \in \mathcal{L}_p(H_1, H_2)$) for $p \in [1, \infty)$ if it is compact and

$$\|T\|_{\mathcal{L}_p} := \|(s_n)_{n\in\mathbb{N}}\|_{\ell^p} < \infty\},$$

where s_n is the nth eigenvalue of $\sqrt{T^*T}$. An operator is called *of trace class* or *Hilbert–Schmidt* if it is of p-th Schatten class for $p = 1$ or $p = 2$, respectively. One can show that $\mathcal{L}_p(H_1, H_2)$ is for each p a Banach space (a Hilbert space for $p = 2$) and an ideal, in the sense that the composition of two operators is of p-Schatten class already if either of them is of p-Schatten class, as soon as the other operator is merely bounded. Because of Hölder's inequality for sequence spaces, $\mathcal{L}_p(H_1, H_2) \subset \mathcal{L}_q(H_1, H_2)$ for all $p \leq q$, and for instance the composition of two Hilbert–Schmidt operators is of trace class.

Roughly speaking, in the following a Banach space is referred to as *lattice* if it carries some order structure that is compatible with its norm. We refer to [17] for a general introduction to this theory, but in the present book we will not deal with any Banach lattices but their most elementary cases, viz spaces of continuous functions over locally compact spaces and L^p-spaces with respect to some σ-finite measure.[1]

Following [19] and [20, Chapter 2] we adopt throughout this book a rather general notion of lattice ideal (more general, e.g., than the one in [18, 23]).

Definition B.5. Given U, V subspaces of $L^p(\Omega, \mathsf{u})$, U is said to be a *lattice ideal* of V if

- $u \in U$ implies $|u| \in V$ and
- $v \operatorname{sgn} u \in U$ provided $u \in U$ and $v \in V$ such that $|v| \leq |u|$.

Then one checks the following, see e.g. [20, Thm. 4.21]. We use the fact that any function $f \in W^{1,p}(I)$ has well-defined boundary values provided I has a nonempty boundary ∂I—in fact, the trace operator is bounded.

Lemma B.6. *Let $I \subset \mathbb{R}$ be an open interval. Let*

$$\mathring{W}^{1,p}(I) := \{f \in W^{1,p}(I) : f_{|\partial I} = 0\}, \qquad 1 \leq p < \infty,$$

and let V be any closed subspace of $W^{1,p}(I)$ that contains $\mathring{W}^{1,p}(I)$. Then for all $p \in [1, \infty)$ $\mathring{W}^{1,p}(I)$ is a lattice ideal of V.

Sobolev spaces can also be defined if one replaces the open interval I by an open domain in $\mathbb{R}^n$, but continuity of $W^{1,p}$-functions is peculiar to the case of $n = 1$.

The proof of Lemma B.3.(2) is based on the Ascoli–Arzelà Theorem. In other cases it may be necessary to prove, more simply, precompactness of subspaces of L^p-spaces—i.e., compactness of the embedding operator from $W^{1,p}(I)$ to $L^q(I)$ for some $p, q \in [1, \infty]$. The classical way of doing so is to apply the *Fréchet–Kolmogorov Theorem*, which has been recently generalized as a consequence of the following *Hanche-Olsen–Holden Lemma*, cf. [11, Lemma 1].

Lemma B.7. *Let (M, d_M) be a metric space. Then M is totally bounded if for all $\varepsilon > 0$ there is $\delta > 0$, a metric space (W, d_W), and a mapping $\Phi : M \to W$ such that*

[1] We stress that this concept of lattice has nothing to do with the *physical* notion of lattice at the core of Example A.11, but we keep this contradictory terminology as we believe that there is very little danger of confusion.

- *$\Phi(M)$ is totally bounded and*
- *for all $x, y \in M$ $d_W(\Phi(x), \Phi(y)) < \delta$ implies $d_M(x, y) < \epsilon$.*

Lemma B.8. *Let $I \subset \mathbb{R}$ be an open interval. Then the following assertions hold.*

(1) If $\partial I \neq \emptyset$, then $C_c^\infty(I)$ is dense in $\mathring{W}^{1,p}(I)$ for all $p \in [1, \infty)$.
(2) There exists $C > 0$ such that

$$\|u\|_{L^2}^3 \le C\|u'\|_{L^2}\|u\|_{L^1}^2, \qquad u \in W^{1,2}(\mathbb{R}) \cap L^1(\mathbb{R}). \tag{B.3}$$

(3) If $I = (\alpha, \beta)$ for some $\alpha, \beta \in \mathbb{R}$, then there exists $C > 0$ such that

$$\|u\|_{L^\infty} \le C\|u'\|_{L^1} + |u(\alpha)|, \qquad u \in W^{1,1}(I). \tag{B.4}$$

(4) If I is bounded, then there exists $C > 0$ such that

$$\|u\|_{L^\infty} \le C\|u'\|_{L^1}, \qquad u \in \mathring{W}^{1,1}(I). \tag{B.5}$$

(5) If I is bounded, then for all $p, q, r \in [1, \infty]$ such that $q \le p$ there exists $C > 0$ such that

$$\|u\|_{L^p} \le C\|u\|_{W^{1,r}}^a \|u\|_{L^q}^{1-a}, \qquad u \in W^{1,r}(I), \tag{B.6}$$

where

$$a := \frac{q^{-1} - p^{-1}}{(1 + q^{-1} - r^{-1})}.$$

In particular,

$$\|u\|_{L^\infty} \le C\|u\|_{W^{1,2}}^{\frac{1}{2}} \|u\|_{L^2}^{\frac{1}{2}}, \qquad u \in W^{1,2}(I). \tag{B.7}$$

Both estimates (B.4)–(B.5) are referred to as *Poincaré inequality*, whereas (B.3) and (B.6) are usually called *Nash inequality* and *Gagliardo-Nirenberg inequality*, respectively. They have important consequences for the long-time behavior of diffusion equations. Observe that the Poincaré inequality shows that

$$(f, g) \mapsto (f'|g')_{L^2(I)} + f(\alpha)\overline{g(\alpha)}$$

defines an equivalent inner product on $\mathring{W}^{1,2}(\alpha, \beta)$.

Example B.9. Consider the operator $S : f \mapsto i\hbar f'$, which in mathematical physics is called the *momentum operator*—in fact, it is the quantum mechanical observable associated to the classical momentum. Then the linear operator S is not bounded on

$L^2(\mathbb{R})$, but is indeed bounded from $W^{1,p}(\mathbb{R})$ to $L^2(\mathbb{R})$. Likewise, $\Delta : f \mapsto f''$ is a bounded linear operator from $H^2(\mathbb{R})$ to $L^2(\mathbb{R})$.

One of the reasons for introducing the Sobolev spaces $W^{k,p}(I)$, in particular for $p = 2$, is that they allow for a convenient operator theoretical setting for studying those operators that are not bounded on usual L^2-spaces, as is typically the case for differential operators; and for solving elliptic problems by means of the following *Lax–Milgram Lemma*, proved in [16].

Lemma B.10. *Let V be a Hilbert space and a a sesquilinear mapping from $V \times V$ to $\mathbb{K}$. Let a be bounded and coercive. Then, for any $\phi \in V'$ there is a unique solution $u =: T\phi \in V$ to $a(u, v) = \langle \phi, v\rangle$—which also satisfies $\|u\| \le \frac{1}{c}\|\phi\|_{V'}$. Moreover, T is an isomorphism from V' to V.*

We conclude this appendix briefly explaining how to treat weakly differentiable vector-valued functions. For the sake of simplicity we focus on the Hilbert case, which is the most interesting for our purposes.

Definition B.11. Let W be a separable Hilbert space and I be an open interval.

(1) The space $L^2(I; W)$ is the set of all weakly measurable functions $f : I \to W$ such that $x \mapsto \|f(x)\|_W$ is of class $L^2(I; \mathbb{R})$, which is a normed space with respect to the norm

$$\|f\|_{L^2(I;W)} := \int_I |f(x)|_W^2 dx.$$

(2) The space $W^{1,2}(I; W)$ is the set

$$W^{1,2}(I;W) := \big\{f \in L^2(I;W) : \exists f' := g \in L^2(I;W) \text{ s.t.} \\ \textstyle\int_I f(x)h'(x)dx = -\int_I g(x)h(x)dx \text{ for all } h \in C_c^\infty(I;\mathbb{R})\big\}, \tag{B.8}$$

which is a normed space with respect to the norm

$$\|f\|_{W^{1,2}(I;W)} := \int_I \left(|f(x)|_W^2 + |f'(x)|_W^2\right) dx.$$

The following has been proved in [5].

Lemma B.12. *Let W be a separable Hilbert space, $p \in (1, \infty)$, and I be an open interval. The following assertions hold.*

(1) If $G : W \to W$ is a Lipschitz continuous mapping and if

- *$G(0) = 0$, or*
- *I is finite,*

then $G \circ f \in W^{1,p}(I; W)$ whenever $f \in W^{1,p}(I; W)$.

(2) *Let W be a complex Hilbert lattice. If $u \in W^{1,p}(I;W)$, then also its real and complex parts* $\operatorname{Re} u, \operatorname{Im} u$ *belong to* $W^{1,p}(I;W)$*, and so do the positive and negative parts* $(\operatorname{Re} u)^+, (\operatorname{Re} u)^-$ *of its real part, with*

$$(\operatorname{Re} u)' = \operatorname{Re}(u'), \qquad ((\operatorname{Re} u)^+)' = \operatorname{Re}(u')\mathbf{1}_{\{u\geq 0\}}.$$

Proof. We start observing that the proof of [3, Prop. 8.5] holds also in the vector-valued case with minor changes. In other words, if $f \in L^p(I;W)$, then $f \in W^{1,p}(I;W)$ is equivalent to the existence of a positive constant C with the property that for all open bounded $\omega \subset I$ and all $h \in \mathbb{R}$ with $|h| \leq$ dist(!, ∂I) one has

$$\int_\omega \|f(x+h) - f(x)\|_W^p dx \leq C|h|^p. \tag{B.9}$$

Assume G to be Lipschitz with constant L. First we note that the estimate

$$\int_\omega \|G(f(x+h)) - G(f(x))\|_W^p dx \leq \int_\omega L^p \|f(x+h) - f(x)\|_W^p dx \leq CL^p|h|^p$$

holds for every $f \in W^{1,p}(\Omega;W)$, since by assumption f satisfies (B.9). It remains to show that $G \circ f \in L^p(\Omega;W)$.

If $G(0) = 0$, it suffices to observe that

$$\begin{aligned}\int_I \|G(f(x))\|_W^p dx &= \int_I \|G(f(x)) - 0\|_W^p dx \\ &= \int_I \|G(f(x)) - G(0)\|_W^p dx \leq L^p \int_I \|f(x)\|_W^p dx < \infty.\end{aligned}$$

Thus $G \circ f \in L^p(I;W)$ and the above criterion applies.

Let now I be bounded. Fix an arbitrary vector $w \in W$ and estimate

$$\begin{aligned}\|G(f(x))\|_W &= \|G(f(x)) - G(w) + G(w)\|_W \\ &\leq L\|f(x) - w\|_W + \|G(w)\|_W \\ &\leq L\|f(x)\|_W + L\|w\|_W + \|G(w)\|_W.\end{aligned}$$

Taking the pth power and integrating on I with respect to x we obtain a finite number, since I has finite measure. □

Remark B.13. The analog of Lemma B.12.(2) does not hold for Sobolev spaces of higher order: Consider $u : (-2,2) \ni x \mapsto x^2 - 1 \in \mathbb{R}$, which belongs to $W^{k,p}(-2,2)$ for any $k \in \mathbb{N}$, $p \in [1,\infty]$, but whose positive part has discontinuous derivative, so that $(u^+)' \notin W^{1,p}(-2,2)$ by Lemma B.3.(1).

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