1 Introduction

Optimization is a staple of mathematical modeling. In this rich framework, we consider a set S called the *search space*—it contains all possible answers to our problem, good and bad—and a *cost function* $f \colon S \to \mathbb{R}$ which associates a cost $f(x)$ to each element x of S. The goal is to find $x \in S$ such that $f(x)$ is as small as possible, that is, a best answer. We write

$$\min_{x \in S} f(x)$$

to represent both the optimization problem and the minimal cost (if it exists). Occasionally, we wish to denote specifically the subset of S for which the minimal cost is attained; the standard notation is

$$\operatorname*{arg\,min}_{x \in S} f(x),$$

bearing in mind that this set might be empty. We will discuss a few simple applications which can be modeled in this form.

Rarely, optimization problems admit an analytical solution. Typically, we need numerical algorithms to (try to) solve them. Often, the best algorithms exploit mathematical structure in S and f.

An important special case arises when S is a linear space such as $\mathbb{R}^n$. Minimizing a function f in $\mathbb{R}^n$ is called *unconstrained optimization* because the variable x is free to move around $\mathbb{R}^n$, unrestricted.

If f is sufficiently differentiable and $\mathbb{R}^n$ is endowed with an inner product (that is, if we make it into a Euclidean space), then we have a notion of gradient and perhaps even a notion of Hessian for f. These objects give us a firm understanding of how f behaves locally around any given point. Famous algorithms such as gradient descent and Newton's method exploit these objects to move around $\mathbb{R}^n$ efficiently in search of a solution.

Notice, however, that the Euclidean structure of $\mathbb{R}^n$ and the smoothness of f are irrelevant to the definition of the optimization problem itself: they are merely structures that we may (and as experience shows, we should) use algorithmically to our advantage.

Subsuming linearity, we focus on *smoothness* as the key structure to exploit: we assume the set S is a *smooth manifold* and the function f is smooth on S. This calls for precise definitions, constructed first in Chapter 3. For a first intuition, one can think of smooth manifolds as surfaces in $\mathbb{R}^n$ that do not have kinks or boundaries, such as a plane, a sphere, a torus, or a hyperboloid.

We could think of optimization over such surfaces as *constrained*, in the sense that x is not allowed to move freely in $\mathbb{R}^n$: it is constrained to remain on the surface. Alternatively, and this is the viewpoint favored here, we can think of this as unconstrained optimization, in a world where the smooth surface is the only thing that exists: like an ant walking on a large ball might feel unrestricted in its movements, aware only of the sphere it lives on; or like the two-dimensional inhabitants of Flatland [Abb84] who find it hard to imagine that there exists such a thing as a third dimension, feeling thoroughly free in their own subspace.

A natural question then is: can we generalize the Euclidean algorithms from unconstrained optimization to handle the broader class of optimization over smooth manifolds? The answer is essentially yes, going back to the 70s [Lue72, Lic79], the 80s [Gab82] and the 90s [Udr94, Smi94, HM96, Rap97, EAS98], and sparking a significant amount of research in the past two decades.

To generalize algorithms such as gradient descent and Newton's method, we need a proper notion of gradient and Hessian on smooth manifolds. In the linear case, this required the introduction of an inner product: a Euclidean structure. In our more general setting, we leverage the fact that smooth manifolds can be linearized locally around every point. The linearization at x is called the *tangent space* at x. By endowing each tangent space with its own inner product (varying smoothly with x, in a sense to be made precise), we construct what is called a *Riemannian structure* on the manifold: it becomes a *Riemannian manifold*.

A Riemannian structure is sufficient to define gradients and Hessians on the manifold, paving the way for optimization. There exist several Riemannian structures on each manifold: our choice may impact algorithmic performance. In that sense, identifying a useful structure is part of the algorithm design—as opposed to being part of the problem formulation, which ended with the definition of the search space (as a crude set) and the cost function.

Chapter 2 covers a few simple applications, mostly to give a sense of how manifolds come up. We then go on to define smooth manifolds in a restricted[1] setting in Chapter 3, where manifolds are *embedded* in a linear space, much like the unit sphere in three-dimensional space. In this context, we define notions of smooth functions, smooth vector fields, gradients and *retractions* (a means to move around on a manifold). These tools are sufficient to design and analyze a first optimization algorithm in Chapter 4: Riemannian gradient descent. As readers progress through these chapters, it is the intention that they also read bits of Chapter 7 from time to time: useful embedded manifolds are studied there in detail. Chapter 5 provides more advanced geometric tools for embedded manifolds, including the notions of Riemannian *connections* and Hessians. These

[1] Some readers may know Whitney's celebrated embedding theorems, which state that any smooth manifold can be embedded in a linear space [BC70, p82]. The mere existence of an embedding, however, is of little use for computation.

are put to good use in Chapter 6 to design and analyze Riemannian versions of Newton's method and the trust-region method.

The linear *embedding space* is useful for intuition, to simplify definitions, and to design tools. Notwithstanding, all the tools and concepts we define in the restricted setting are *intrinsic*, in the sense that they are well defined regardless of the embedding space. We make this precise much later, in Chapter 8, where all the tools from Chapters 3 and 5 are redefined in the full generality of standard treatments of differential geometry. This is also the time to discuss topological issues to some extent. Generality notably makes it possible to discuss a more abstract class of manifolds called *quotient manifolds* in Chapter 9. They offer a beautiful way to harness symmetry, so common in applications.

In closing, Chapter 10 offers a limited treatment of more advanced geometric tools such as the Riemannian distance, geodesics, the exponential map and its inverse, parallel transports and transporters, notions of Lipschitz continuity, finite differences, and covariant differentiation of tensor fields. Then, Chapter 11 covers elementary notions of convexity on Riemannian manifolds with simple implications for optimization. This topic has been around since the 90s, and has been gaining traction in research lately.

More than 150 years ago, Riemann invented a new kind of geometry for the abstract purpose of understanding curvature in high-dimensional spaces. Today, this geometry plays a central role in the development of efficient algorithms to tackle technological applications Riemann himself—arguably—could have never envisioned. Through this book, I invite you to enjoy this singularly satisfying success of mathematics, with an eye to turning geometry into algorithms.

2 Simple examples

Before formally defining what manifolds are, and before introducing any particular algorithms, this chapter surveys simple problems that are naturally modeled as optimization on manifolds. These problems are motivated by applications in various scientific and technological domains. We introduce them chiefly to illustrate how manifolds arise and to motivate the mathematical abstractions in subsequent chapters.

The first example leads to optimization on an affine subspace: it falls within the scope of optimization on manifolds, but one can also handle it with classical tools. Subsequently, we encounter optimization on spheres, products of spheres, orthonormal matrices, the set of all linear subspaces, rotation matrices, fixed-rank matrices, positive definite matrices and certain quadratic surfaces. Through those, we get a glimpse of the wide reach of optimization on manifolds.

Below, we use a few standard concepts from linear algebra and calculus that are revisited in Section 3.1.

2.1 Sensor network localization from directions: an affine subspace

Consider n sensors located at unknown positions $t_1, \ldots, t_n$ in $\mathbb{R}^d$. We aim to locate the sensors, that is, estimate the positions t_i, based on some directional measurements. Specifically, for each pair of sensors (i, j) corresponding to an edge of a graph G, we receive a noisy measurement of the direction from t_j to t_i:

$$v_{ij} \approx \frac{t_i - t_j}{\|t_i - t_j\|},$$

where $\|x\| = \sqrt{x_1^2 + \cdots + x_d^2}$ is the Euclidean norm on $\mathbb{R}^d$ induced by the inner product $\langle u, v\rangle = u^\top v = u_1 v_1 + \cdots + u_d v_d$.

There are two fundamental ambiguities in this task. First, directional measurements reveal nothing about the global location of the sensors: translating the sensors as a whole does not affect pairwise directions. Thus, we may assume without loss of generality that the sensors are centered:

$$t_1 + \cdots + t_n = 0.$$

Second, the measurements reveal nothing about the global scale of the sensor arrangement. Specifically, scaling all positions t_i by a scalar $\alpha > 0$ as αt_i has no effect on the directions separating the sensors, so that the true scale cannot be recovered from the measurements. It is thus legitimate to fix the scale arbitrarily, to break symmetry. One fruitful way is to assume the following [HLV18]:

$$\sum_{(i,j)\in G} \langle t_i - t_j, v_{ij} \rangle = 1.$$

Indeed, if this constraint holds for some set of locations $t_1, \ldots, t_n$, then it does not hold for locations $\alpha t_1, \ldots, \alpha t_n$ unless $\alpha = 1$.

Given a tentative estimator $\hat{t}_1, \ldots, \hat{t}_n \in \mathbb{R}^d$ for the locations, we may assess its compatibility with the measurement v_{ij} by computing

$$\|(\hat{t}_i - \hat{t}_j) - \left\langle \hat{t}_i - \hat{t}_j, v_{ij} \right\rangle v_{ij}\|.$$

Indeed, if $\hat{t}_i - \hat{t}_j$ and v_{ij} are aligned in the same direction, this evaluates to zero. Otherwise, it evaluates to a positive number, growing as alignment degrades. Combined with the symmetry-breaking conditions, this suggests the following formulation for sensor network localization from direction measurements:

$$\begin{aligned} &\min_{\hat{t}_1,\ldots,\hat{t}_n \in \mathbb{R}^d} \sum_{(i,j)\in G} \|(\hat{t}_i - \hat{t}_j) - \left\langle \hat{t}_i - \hat{t}_j, v_{ij} \right\rangle v_{ij}\|^2 \\ &\text{subject to } \; \hat{t}_1 + \cdots + \hat{t}_n = 0 \; \text{ and } \sum_{(i,j)\in G} \left\langle \hat{t}_i - \hat{t}_j, v_{ij} \right\rangle = 1. \end{aligned}$$

The role of the second constraint is clear: it excludes $\hat{t}_1 = \cdots = \hat{t}_n = 0$, which would otherwise be optimal.

Grouping the variables as the columns of a matrix, we find that the search space for this problem is an affine subspace of $\mathbb{R}^{d\times n}$: this is a *linear manifold.* It is also an *embedded submanifold* of $\mathbb{R}^{d\times n}$. Hence, it falls within our framework.

With the simple cost function as above, this problem is in fact a convex quadratic minimization problem on an affine subspace. As such, it admits an explicit solution which merely requires solving a linear system. Optimization algorithms can be used to solve this system implicitly. More importantly, the power of optimization algorithms lies in the flexibility that they offer: alternative cost functions may be used to improve robustness against specific noise models for example, and those require more general algorithms [HLV18].

2.2 Single extreme eigenvalue or singular value: spheres

Let $A \in \mathbb{R}^{n\times n}$ be a symmetric matrix: $A = A^\top$. By the spectral theorem, A admits n real eigenvalues $\lambda_1 \leq \cdots \leq \lambda_n$ and corresponding real, orthonormal eigenvectors $v_1, \ldots, v_n \in \mathbb{R}^n$, where orthonormality is assessed with respect to the standard inner product over $\mathbb{R}^n$: $\langle u, v \rangle = u^\top v$.

For now, we focus on computing one extreme eigenpair of A: (λ_1, v_1) or (λ_n, v_n)

will do. Let $\mathbb{R}^n_*$ denote the set of nonzero vectors in $\mathbb{R}^n$. It is well known that the *Rayleigh quotient*,

$$r\colon \mathbb{R}^n_* \to \mathbb{R}\colon x \mapsto r(x) = \frac{\langle x, Ax\rangle}{\langle x, x\rangle},$$

attains its extreme values when x is aligned with $\pm v_1$ or $\pm v_n$, and that the corresponding value of the quotient is λ_1 or λ_n. We will rediscover such properties through the prism of optimization on manifolds as a running example in this book. One can gain some insight by checking that $r(v_i) = \lambda_i$.

Say we are interested in the smallest eigenvalue, λ_1. Then, we must solve the following optimization problem:

$$\min_{x \in \mathbb{R}^n_*} \frac{\langle x, Ax\rangle}{\langle x, x\rangle}.$$

The set $\mathbb{R}^n_*$ is open in $\mathbb{R}^n$: it is an *open submanifold* of $\mathbb{R}^n$. Optimization over an open set has its challenges (more on this later). Fortunately, we can easily circumvent these issues in this instance.

Since the Rayleigh quotient is invariant to scaling, that is, since $r(\alpha x) = r(x)$ for all nonzero real α, we may fix the scale arbitrarily. Given the denominator of r, one particularly convenient way is to restrict our attention to unit-norm vectors: $\|x\|^2 = \langle x, x\rangle = 1$. The set of such vectors is the *unit sphere* in $\mathbb{R}^n$:

$$\mathrm{S}^{n-1} = \{x \in \mathbb{R}^n : \|x\| = 1\}.$$

This is an *embedded submanifold* of $\mathbb{R}^n$. Our problem becomes:

$$\min_{x \in \mathrm{S}^{n-1}} \langle x, Ax\rangle. \tag{2.1}$$

This is perhaps the simplest non-trivial instance of an optimization problem on a manifold: we use it recurringly to illustrate concepts as they occur.

Similarly to the above, we may compute the largest singular value of a matrix $M \in \mathbb{R}^{m\times n}$ together with associated left- and right-singular vectors by solving

$$\max_{x \in \mathrm{S}^{m-1}, y \in \mathrm{S}^{n-1}} \langle x, My\rangle. \tag{2.2}$$

This is the basis of *principal component analysis*: see also Section 2.4. The search space is a Cartesian product of two spheres. This too is a manifold; specifically, an embedded submanifold of $\mathbb{R}^m \times \mathbb{R}^n$. In general:

Products of manifolds are manifolds.

This is an immensely useful property.

2.3 Dictionary learning: products of spheres

JPEG and its more recent version JPEG 2000 are some of the most commonly used compression standards for photographs. At their core, these algorithms rely on basis expansions: discrete cosine transforms for JPEG, and wavelet transforms for JPEG 2000. That is, an image (or rather, each patch of the image) is written as a linear combination of a fixed collection of basis images. To fix notation, say an image is represented as a vector $y \in \mathbb{R}^d$ (its pixels rearranged into a single column vector) and the basis images are $b_1, \ldots, b_d \in \mathbb{R}^d$ (each of unit norm). There exists a unique set of coordinates $c \in \mathbb{R}^d$ such that:

$$y = c_1 b_1 + \cdots + c_d b_d.$$

Since the basis images are fixed (and known to anyone creating or reading image files in this format), it is equivalent to store y or c.

The basis is designed carefully with two goals in mind. First, the transform between y and c should be fast to compute (one good starting point to that effect is orthogonality). Second, images encountered in practice should lead to many of the coefficients c_i being zero, or close to zero. Indeed, to recover y, it is only necessary to record the nonzero coefficients. To compress further, we may also decide not to store the small coefficients: if so, y can still be reconstructed approximately. Beyond compression, another benefit of sparse expansions is that they can reveal structural information about the contents of the image.

In *dictionary learning*, we focus on the second goal. As a key departure from the above, the idea here is not to design a basis by hand, but rather to learn a good basis from data automatically. This way, we may exploit structural properties of images that come up in a particular application. For example, it may be the case that photographs of faces can be expressed more sparsely in a dedicated basis as compared to a standard wavelet basis. Pushing this idea further, we relax the requirement of identifying a basis, instead allowing ourselves to pick more than d images for our expansions. The collection of images $b_1, \ldots, b_n \in \mathbb{R}^d$ forms a *dictionary*. Its elements are called *atoms*, and they normally span $\mathbb{R}^d$ in an overcomplete way, meaning any image y can be expanded into a linear combination of atoms in more than one way. The aim is that at least one of these expansions should be sparse, or have many small coefficients. For the magnitudes of coefficients to be meaningful, we further require all atoms to have the same norm: $\|b_i\| = 1$ for all i.

Thus, given a collection of k images $y_1, \ldots, y_k \in \mathbb{R}^d$, the task in dictionary learning is to find atoms $b_1, \ldots, b_n \in \mathbb{R}^d$ such that (as much as possible) each image y_i is a sparse linear combination of the atoms. Collect the input images as the columns of a data matrix $Y \in \mathbb{R}^{d \times k}$, and the atoms into a matrix $D \in \mathbb{R}^{d \times n}$ (to be determined). Expansion coefficients for the images in this dictionary form the columns of a matrix $C \in \mathbb{R}^{n \times k}$ so that

$$Y = DC.$$

Typically, many choices of C are possible. We aim to pick D such that there exists a valid (or approximately valid) choice of C with numerous zeros. Let $\|C\|_0$ denote the number of entries of C different from zero. Then, one possible formulation of dictionary learning balances both aims with a parameter $\lambda > 0$

as (with $b_1, \ldots, b_n$ the columns of the dictionary matrix D):

$$\min_{D \in \mathbb{R}^{d \times n}, C \in \mathbb{R}^{n \times k}} \|Y - DC\|^2 + \lambda \|C\|_0 \qquad (2.3)$$
$$\text{subject to } \|b_1\| = \cdots = \|b_n\| = 1.$$

The matrix norm $\|\cdot\|$ is the Frobenius norm, induced by the standard inner product $\langle U, V \rangle = \mathrm{Tr}(U^\top V)$.

Evidently, allowing the dictionary to be overcomplete ($n > d$) helps sparsity. An extreme case is to set $n = k$, in which case an optimal solution consists in letting D be Y with normalized columns. Then, each image can be expressed with a single nonzero coefficient (C is diagonal). This is useless of course, if only because both parties of the communication must have access to the (possibly huge) dictionary, and because this choice may generalize poorly when presented with new images. Interesting scenarios involve n much smaller than k.

The search space for D is a product of several spheres, which is an embedded submanifold of $\mathbb{R}^{d \times n}$ called the *oblique manifold*:

$$\mathrm{OB}(d, n) = (\mathrm{S}^{d-1})^n = \left\{ X \in \mathbb{R}^{d \times n} : \mathrm{diag}(X^\top X) = \mathbf{1} \right\},$$

where $\mathbf{1} \in \mathbb{R}^n$ is the all-ones vector and $\mathrm{diag}\colon \mathbb{R}^{n \times n} \to \mathbb{R}^n$ extracts the diagonal entries of a matrix. The search space in C is the linear manifold $\mathbb{R}^{n \times k}$. Overall, the search space of the dictionary learning optimization problem is

$$\mathrm{OB}(d, n) \times \mathbb{R}^{n \times k},$$

which is an embedded submanifold of $\mathbb{R}^{d \times n} \times \mathbb{R}^{n \times k}$.

We note in closing that the cost function in (2.3) is discontinuous because of the term $\|C\|_0$, making it hard to optimize. A standard reformulation replaces the culprit with $\|C\|_1$: the sum of absolute values of the entries of C. This is continuous but nonsmooth. A possible further step then is to smooth the cost function, for example exploiting that $|x| \approx \sqrt{x^2 + \varepsilon^2}$ or $|x| \approx \varepsilon \log(e^{x/\varepsilon} + e^{-x/\varepsilon})$ for small $\varepsilon > 0$: these are standard tricks.

Regardless of changes to the cost function, the manifold $\mathrm{OB}(d, n)$ is nonconvex, so that finding a global optimum for dictionary learning as stated above is challenging: see work by Sun et al. [SQW17] for some guarantees.

2.4 Principal component analysis: Stiefel and Grassmann

Let $x_1, \ldots, x_n \in \mathbb{R}^d$ represent a large collection of centered data points in a d-dimensional linear space. We may think of it as a cloud of points. It may be the case that this cloud lies on or near a low-dimensional subspace of $\mathbb{R}^d$, and it may be distributed anisotropically in that subspace, meaning it shows more variation along some directions than others. One of the pillars of data analysis is to determine the main directions of variation of the data. This goes by the name of principal component analysis (PCA), which we encountered in Section 2.2.

One way to think of a main direction of variation, called a *principal component*, is as a vector $u \in \mathrm{S}^{d-1}$ such that projecting the data points to the one-dimensional subspace spanned by u 'preserves most of the variance.' Specifically, let $X \in \mathbb{R}^{d\times n}$ be the matrix whose columns are the data points and let $uu^\top$ be the orthogonal projector from $\mathbb{R}^d$ to the span of u. We wish to maximize the following for $u \in \mathrm{S}^{d-1}$:

$$\sum_{i=1}^{n} \|uu^\top x_i\|^2 = \|uu^\top X\|^2 = \langle X^\top uu^\top, X^\top uu^\top\rangle = \langle XX^\top u, u\rangle.$$

We recognize the Rayleigh quotient of the matrix $XX^\top$ to be maximized for u over S^{d-1} (Section 2.2). An optimal solution is given by a dominant eigenvector of $XX^\top$, or equivalently by a dominant left singular vector of X.

Let $u_1 \in \mathrm{S}^{d-1}$ be a principal component. We would like to find a second one. That is, we aim to find $u_2 \in \mathrm{S}^{d-1}$, *orthogonal to* u_1, such that projecting the data to the subspace spanned by u_1 and u_2 preserves the most variance. The orthogonal projector to that subspace is $u_1u_1^\top + u_2u_2^\top$. We maximize

$$\|(u_1u_1^\top + u_2u_2^\top)X\|^2 = \langle XX^\top u_1, u_1\rangle + \langle XX^\top u_2, u_2\rangle$$

over $u_2 \in \mathrm{S}^{d-1}$ with $u_2^\top u_1 = 0$. The search space for u_2 is an embedded submanifold of $\mathbb{R}^d$: it is a unit sphere in the subspace orthogonal to u_1.

It is often more convenient to optimize for u_1 and u_2 simultaneously rather than sequentially. Then, since the above cost function is symmetric in u_1 and u_2, as is the constraint $u_2^\top u_1 = 0$, we add weights to the two terms to ensure u_1 captures a principal component and u_2 captures a second principal component:

$$\max_{u_1,u_2\in\mathrm{S}^{d-1}, u_2^\top u_1=0} \alpha_1\langle XX^\top u_1, u_1\rangle + \alpha_2\langle XX^\top u_2, u_2\rangle,$$

with $\alpha_1 > \alpha_2 > 0$ arbitrary.

More generally, aiming for k principal components, we look for a matrix $U \in \mathbb{R}^{d\times k}$ with k orthonormal columns $u_1, \ldots, u_k \in \mathbb{R}^d$. The set of such matrices is called the *Stiefel manifold*:

$$\mathrm{St}(d,k) = \{U \in \mathbb{R}^{d\times k} : U^\top U = I_k\},$$

where I_k is the identity matrix of size k. It is an embedded submanifold of $\mathbb{R}^{d\times k}$. The orthogonal projector to the subspace spanned by the columns of U is $UU^\top$. Hence, PCA amounts to solving the problem:

$$\max_{U\in\mathrm{St}(d,k)} \sum_{i=1}^{k} \alpha_i\langle XX^\top u_i, u_i\rangle = \max_{U\in\mathrm{St}(d,k)} \langle XX^\top U, UD\rangle, \tag{2.4}$$

where $D \in \mathbb{R}^{k\times k}$ is diagonal with diagonal entries $\alpha_1 > \cdots > \alpha_k > 0$.

It is well known that collecting k top eigenvectors of $XX^\top$ (or, equivalently, k top left singular vectors of X) yields a global optimum of (2.4), meaning this optimization problem can be solved efficiently using tools from numerical linear algebra. Still, the optimization perspective offers significant flexibility that standard linear algebra algorithms cannot match. Specifically, within an optimization framework, it is possible to revisit the variance criterion by changing the cost function. This allows one to promote sparsity or robustness against outliers, for example to develop variants such as sparse PCA [dBEG08, JNRS10] and robust PCA [MT11, GZAL14, MZL19, NNSS20]. There may also be computational advantages, for example in tracking and online models where the dataset changes or grows with time: it may be cheaper to update a previously computed good estimator using few optimization steps than to run a complete eigenvalue or singular value decomposition anew.

If the top k principal components are of interest but their ordering is not, then we do not need the weight matrix D. In this scenario, we are seeking an orthonormal basis U for a k dimensional subspace of $\mathbb{R}^d$ such that projecting the data to that subspace preserves as much of the variance as possible. This description makes it clear that the particular basis is irrelevant: only the selected subspace matters. This is apparent in the cost function,

$$f(U) = \langle XX^\top U, U\rangle,$$

which is invariant under orthogonal transformations. Specifically, for all Q in the orthogonal group

$$\mathrm{O}(k) = \{Q \in \mathbb{R}^{k\times k} : Q^\top Q = I_k\},$$

we have $f(UQ) = f(U)$. This induces an *equivalence relation*[1] $\sim$ on the Stiefel manifold:

$$U \sim V \qquad\qquad \iff \qquad\qquad V = UQ \text{ for some } Q \in \mathrm{O}(k).$$

This equivalence relation partitions $\mathrm{St}(d,k)$ into *equivalence classes*:

$$[U] = \{V \in \mathrm{St}(d,k) : U \sim V\} = \{UQ : Q \in \mathrm{O}(k)\}.$$

The set of equivalence classes is called the *quotient set*:

$$\mathrm{St}(d,k)/\!\sim\; = \mathrm{St}(d,k)/\mathrm{O}(k) = \{[U] : U \in \mathrm{St}(d,k)\}.$$

Importantly, $U, V \in \mathrm{St}(d,k)$ are equivalent if and only if their columns span the same subspace of $\mathbb{R}^d$. In other words: the quotient set is in one-to-one correspondence with the set of subspaces of dimension k in $\mathbb{R}^d$. With the right geometry, the latter is called the *Grassmann manifold*:

$$\mathrm{Gr}(d,k) = \{ \text{ subspaces of dimension } k \text{ in } \mathbb{R}^d \} \equiv \mathrm{St}(d,k)/\mathrm{O}(k),$$

where the symbol $\equiv$ reads "is equivalent to" (context indicates in what sense). As defined here, the Grassmann manifold is a *quotient manifold*. This type of

[1] Recall that an equivalence relation $\sim$ on a set $\mathcal{M}$ is a reflexive ($a \sim a$), symmetric ($a \sim b \iff b \sim a$) and transitive ($a \sim b$ and $b \sim c \implies a \sim c$) binary relation. The equivalence class $[a]$ is the set of elements of $\mathcal{M}$ that are equivalent to a. Each element of $\mathcal{M}$ belongs to exactly one equivalence class.

manifold is more abstract than embedded submanifolds, but we can still develop numerically efficient tools to work with them.

Within our framework, computing the dominant eigenspace of dimension k of the matrix $XX^\top$ can be written as:

$$\max_{[U]\in \mathrm{Gr}(d,k)} \langle XX^\top U, U\rangle.$$

The cost function is well defined over $\mathrm{Gr}(d,k)$ since it depends only on the equivalence class of U, not on U itself.

Going back to (2.4), we note in passing that k top left and right singular vectors of a matrix $M \in \mathbb{R}^{m\times n}$ can be computed by solving the following problem on a product of Stiefel manifolds (this and (2.4) are sometimes called *Brockett cost functions*):

$$\max_{U\in \mathrm{St}(m,k), V\in \mathrm{St}(n,k)} \langle MV, UD\rangle,$$

where $D = \mathrm{diag}(\alpha_1,\ldots,\alpha_k)$ with arbitrary $\alpha_1 > \cdots > \alpha_k > 0$ as above.

A book by Trendafilov and Gallo provides more in-depth discussion of applications of optimization on manifolds to data analysis [TG21].

2.5 Synchronization of rotations: special orthogonal group

In structure from motion (SfM), the 3D structure of an object is to be reconstructed from several 2D images of it. For example, in the paper *Building Rome in a Day* [ASS+09], the authors automatically construct a model of the Colosseum from over 2000 photographs freely available on the Internet. Because the pictures are acquired from an unstructured source, one of the steps in the reconstruction pipeline is to estimate camera locations and *pose*. The pose of a camera is its orientation in space.

In single particle reconstruction through cryo electron microscopy, an electron microscope is used to produce 2D tomographic projections of biological objects such as proteins and viruses. Because shape is a determining factor of function, the goal is to estimate the 3D structure of the object from these projections. Contrary to X-ray crystallography (another fundamental tool of structural biology), the orientations of the objects in the individual projections are unknown. In order to estimate the structure, a useful step is to estimate the individual orientations (though high noise levels do not always allow it, in which case alternative statistical techniques must be used.)

Mathematically, orientations correspond to rotations of $\mathbb{R}^3$. Rotations in $\mathbb{R}^d$ can be represented with orthogonal matrices:

$$\mathrm{SO}(d) = \{R \in \mathbb{R}^{d\times d} : R^\top R = I_d \text{ and } \det(R) = +1\}.$$

The determinant condition excludes reflections of $\mathbb{R}^d$. The set $\mathrm{SO}(d)$ is the *special* *orthogonal group*: it is both a group (in the mathematical sense of the term) and a manifold (an embedded submanifold of $\mathbb{R}^{d\times d}$)—it is a *Lie group*.

In both applications described above, similar images or projections can be compared to estimate relative orientations. *Synchronization of rotations* is a mathematical abstraction of the ensuing task. It consists in estimating n individual rotation matrices,

$$R_1, \ldots, R_n \in \mathrm{SO}(d),$$

from pairwise relative rotation measurements: for some pairs (i, j) corresponding to the edges of a graph G, we observe a noisy version of $R_i R_j^{-1}$. Let $H_{ij} \in \mathrm{SO}(d)$ denote such a measurement. Then, one possible formulation of synchronization of rotations is:

$$\min_{\hat{R}_1,\ldots,\hat{R}_n \in \mathrm{SO}(d)} \sum_{(i,j)\in G} \|\hat{R}_i - H_{ij}\hat{R}_j\|^2.$$

This is an optimization problem over $\mathrm{SO}(d)^n$, which is a manifold.

This also comes up in *simultaneous localization and mapping* (SLAM), whereby a robot must simultaneously map its environment and locate itself in it as it moves around [RDTEL21]. An important aspect of SLAM is to keep track of the robot's orientation accurately, by integrating all previously acquired information to correct estimator drift.

2.6 Low-rank matrix completion: fixed-rank manifold

Let $M \in \mathbb{R}^{m\times n}$ be a large matrix of interest. Given some of its entries, our task is to estimate the whole matrix. A commonly cited application for this setup is that of recommender systems, where row i corresponds to a user, column j corresponds to an item (a movie, a book…) and entry M_{ij} indicates how much user i appreciates item j: positive values indicate appreciation, zero is neutral, and negative values indicate dislike. The known entries may be collected from user interactions. Typically, most entries are unobserved. Predicting the missing values may be helpful to automate personalized recommendations.

Of course, without further knowledge about how the entries of the matrix are related, the completion task is ill-posed. Hope comes from the fact that certain users share similar traits, so that what one user likes may be informative about what another, similar user may like. In the same spirit, certain items may be similar enough that whole groups of users may feel similarly about them. One mathematically convenient way to capture this idea is to assume M has (approximately) low rank. The rationale is as follows: if M has rank r, then it can be factored as

$$M = LR^\top,$$

where $L \in \mathbb{R}^{m\times r}$ and $R \in \mathbb{R}^{n\times r}$ are full-rank factor matrices. Row i of L, ℓ_i, attributes r numbers to user i, while the jth row of R, r_j, attributes r numbers to item j. Under the low-rank model, the rating of user i for item j is $M_{ij} = \langle \ell_i, r_j \rangle$. One interpretation is that there are r latent features (these could be movie genres for example): a user has some positive or negative appreciation for each feature, and an item has traits aligned with or in opposition to these features; the rating is obtained as the inner product of the two feature vectors.

Under this model, predicting the user ratings for all items amounts to *low-rank matrix completion*. Let Ω denote the set of pairs (i, j) such that M_{ij} is observed. Allowing for noise in the observations and inaccuracies in the model, we aim to solve

$$\begin{aligned} &\min_{X \in \mathbb{R}^{m\times n}} \sum_{(i,j)\in\Omega} (X_{ij} - M_{ij})^2 \\ &\text{subject to } \operatorname{rank}(X) = r. \end{aligned}$$

The search space for this optimization problem is the set of matrices of a given size and rank:

$$\mathbb{R}_r^{m\times n} = \{X \in \mathbb{R}^{m\times n} : \operatorname{rank}(X) = r\}.$$

This set is an embedded submanifold of $\mathbb{R}^{m\times n}$ which is frequently useful in machine learning applications.

Another use for this manifold is solving high-dimensional matrix equations that may come up in systems and control applications: aiming for a low-rank solution may be warranted in certain settings, and exploiting this can lower the computational burden substantially. Yet another context where optimization over low-rank matrices occurs is in completing and denoising approximately separable bivariate functions based on sampled values [Van10, Van13, MV13].

The same set can also be endowed with other geometries, that is, it can be made into a manifold in other ways. For example, exploiting the factored form more directly, note that any matrix in $\mathbb{R}_r^{m\times n}$ admits a factorization as $LR^\top$ with both L and R of full rank r. This correspondence is not one-to-one however, since the pairs (L, R) and $(LJ^{-1}, RJ^\top)$ map to the same matrix in $\mathbb{R}_r^{m\times n}$ for all invertible matrices J: they are equivalent. Similarly to the Grassmann manifold, this leads to a definition of $\mathbb{R}_r^{m\times n}$ as a quotient manifold instead of an embedded submanifold. Many variations on this theme are possible, some of them more useful than others depending on the application [Mey11, Mis14].

The set $\mathbb{R}_r^{m\times n}$ is not closed in $\mathbb{R}^{m\times n}$, which may create difficulties for optimization. The closure of the set corresponds to all matrices of rank at most r (rather than exactly equal to r). That set is not a manifold, but it can be smoothly parameterized by a manifold in several ways [LKB22b]. One particularly simple way is through the map $(L, R) \mapsto LR^\top$ where L and R are allowed to be rank deficient.

2.7 Gaussian mixture models: positive definite matrices

A common model in machine learning assumes data $x_1, \ldots, x_n \in \mathbb{R}^d$ are sampled independently from a *mixture of* K *Gaussians*, that is, each data point is sampled from a probability distribution with density of the form

$$f(x) = \sum_{k=1}^{K} w_k \frac{1}{\sqrt{2\pi \det(\Sigma_k)}} e^{-\frac{(x-\mu_k)^\top \Sigma_k^{-1}(x-\mu_k)}{2}},$$

where the centers $\mu_1, \ldots, \mu_K \in \mathbb{R}^d$, covariances $\Sigma_1, \ldots, \Sigma_K \in \mathrm{Sym}(d)^+$ and mixing probabilities $(w_1, \ldots, w_K) \in \Delta_+^{K-1}$ are to be determined. We use the following notation:

$$\mathrm{Sym}(d)^+ = \{X \in \mathbb{R}^{d\times d} : X = X^\top \text{ and } X \succ 0\}$$

for symmetric, positive definite matrices of size d, and

$$\Delta_+^{K-1} = \{w \in \mathbb{R}^K : w_1, \ldots, w_K > 0 \text{ and } w_1 + \cdots + w_K = 1\}$$

for the positive part of the simplex, that is, the set of non-vanishing discrete probability distributions over K objects. In this model, with probability w_k, a point x is sampled from the kth Gaussian, with mean μ_k and covariance Σ_k. The aim is only to estimate the parameters, not to estimate which Gaussian each point x_i was sampled from.

For a given set of observations $x_1, \ldots, x_n$, a maximum likelihood estimator solves:

$$\max_{\substack{\hat\mu_1,\ldots,\hat\mu_K \in \mathbb{R}^d, \\ \hat\Sigma_1,\ldots,\hat\Sigma_K \in \mathrm{Sym}(d)^+, \\ w \in \Delta_+^{K-1}}} \sum_{i=1}^{n} \log\left(\sum_{k=1}^{K} w_k \frac{1}{\sqrt{2\pi \det(\Sigma_k)}} e^{-\frac{(x_i-\mu_k)^\top \Sigma_k^{-1}(x_i-\mu_k)}{2}} \right). \tag{2.5}$$

This is an optimization problem over $\mathbb{R}^{d\times K} \times (\mathrm{Sym}(d)^+)^K \times \Delta_+^{K-1}$, which can be made into a manifold because $\mathrm{Sym}(d)^+$ and Δ_+^{K-1} can be given a manifold structure.

The direct formulation of maximum likelihood estimation for Gaussian mixture models in (2.5) is, however, not computationally favorable. See [HS15] for a beneficial reformulation, still on a manifold.

2.8 Smooth semidefinite programs

Semidefinite programs (SDPs) are optimization problems of the form

$$\min_{X \in \mathrm{Sym}(n)} \langle C, X\rangle \qquad \text{subject to} \qquad \mathcal{A}(X) = b \qquad \text{and} \qquad X \succeq 0, \tag{2.6}$$

where $\mathrm{Sym}(n)$ is the space of real, symmetric matrices of size $n \times n$, $\langle A, B\rangle = \mathrm{Tr}(A^\top B)$, $\mathcal{A} \colon \mathrm{Sym}(n) \to \mathbb{R}^m$ is a linear map defined by m symmetric matrices $A_1, \ldots, A_m$ as $\mathcal{A}(X)_i = \langle A_i, X\rangle$, and $X \succeq 0$ means X is positive semidefinite.

SDPs are convex and they can be solved to global optimality in polynomial time using interior point methods [Nes18, §5.4.4]. Still, handling the positive semidefiniteness constraint $X \succeq 0$ and the dimensionality of the problem (namely, the $\frac{n(n+1)}{2}$ variables required to define X) both pose significant computational challenges for large n.

A popular way to address both issues is the Burer–Monteiro approach [BM05], which consists in factorizing X as $X = YY^\top$ with $Y \in \mathbb{R}^{n\times p}$: the number p of columns of Y is a parameter. Notice that X is now automatically positive semidefinite. If $p \geq n$, the SDP can be rewritten equivalently as

$$\min_{Y \in \mathbb{R}^{n\times p}} \langle CY, Y\rangle \qquad \text{subject to} \qquad \mathcal{A}(YY^\top) = b. \tag{2.7}$$

If $p < n$, this corresponds to the SDP with the additional constraint $\operatorname{rank}(X) \leq p$. There is a computational advantage to taking p as small as possible. Interestingly, if the set of matrices X that are feasible for the SDP is compact, then the *Pataki–Barvinok bound* [Pat98, Bar95] provides that at least one of the global optimizers of the SDP has rank r such that $\frac{r(r+1)}{2} \leq m$. In other words: assuming compactness, the Burer–Monteiro formulation (2.7) is *equivalent* to the original SDP so long as p satisfies $\frac{p(p+1)}{2} \geq m$. This is already the case for $p = O(\sqrt{m})$, which may be significantly smaller than n.

The positive semidefiniteness constraint disappeared, and the dimensionality of the problem went from $O(n^2)$ to np—a potentially appreciable gain. Yet, we lost something important along the way: the Burer–Monteiro problem is not convex. It is not immediately clear how to solve it.

The search space of the Burer–Monteiro problem is the set of feasible Y:

$$\mathcal{M} = \{Y \in \mathbb{R}^{n\times p} : \mathcal{A}(YY^\top) = b\}. \tag{2.8}$$

Assume the map $Y \mapsto \mathcal{A}(YY^\top)$ has the property that its differential at all Y in $\mathcal{M}$ has rank m. Then, $\mathcal{M}$ is an embedded submanifold of $\mathbb{R}^{n\times p}$. In this special case, we may try to solve the Burer–Monteiro problem through optimization over that manifold. It turns out that non-convexity is mostly benign in that scenario, in a precise sense [BVB19]:

If $\mathcal{M}$ is compact and $\frac{p(p+1)}{2} > m$, then, for a generic cost matrix C, the smooth optimization problem $\min_{Y\in\mathcal{M}} \langle CY, Y\rangle$ has no spurious local minima, in the sense that any point Y which satisfies first- and second-order necessary optimality conditions is a global optimum.

(Necessary optimality conditions are detailed in Sections 4.2 and 6.1.) Additionally, these global optima map to global optima of the SDP through $X = YY^\top$. This suggests that smooth-and-compact SDPs may be solved to global optimality via optimization on manifolds. The requirement that $\mathcal{M}$ be a regularly defined smooth manifold is not innocuous, but it is satisfied in a number of interesting applications.

There has been a lot of work on this front in recent years, including the early work by Burer and Monteiro [BM03, BM05], the first manifold-inspired perspective by Journée et al. [JBAS10], qualifications of the benign non-convexity at the Pataki–Barvinok threshold [BVB16, BVB19] and below in special cases [BBV16], a proof that p cannot be set much lower than that threshold in general [WW20], smoothed analyses to assess whether points which satisfy necessary optimality conditions approximately are also approximately optimal [BBJN18, PJB18, CM19] and extensions to accommodate scenarios where $\mathcal{M}$ is not a smooth manifold but, more generally, a real algebraic variety [BBJN18, Cif21]. See all these references for applications, including Max-Cut, community detection, the trust-region subproblem, synchronization of rotations and more.

3 Embedded geometry: first order

Our goal is to develop optimization algorithms to solve problems of the form

$$\min_{x \in \mathcal{M}} f(x), \tag{3.1}$$

where $\mathcal{M}$ is a smooth and possibly nonlinear space, and $f \colon \mathcal{M} \to \mathbb{R}$ is a smooth cost function. In order to do so, our first task is to clarify what we mean by a "smooth space," and a "smooth function" on such a space. Then, we need to develop any tools required to construct optimization algorithms in this setting. Let us start with a bird's-eye view of what this entails, and formalize later on.

For smoothness of $\mathcal{M}$, our model space is the unit sphere in $\mathbb{R}^d$:

$$\mathrm{S}^{d-1} = \{x \in \mathbb{R}^d : x^\top x = 1\}. \tag{3.2}$$

Intuitively, we think of S^{d-1} as a smooth nonlinear space in $\mathbb{R}^d$. Our definitions below are compatible with this intuition: we call S^{d-1} an *embedded submanifold* of $\mathbb{R}^d$.

An important element in these definitions is to capture the idea that S^{d-1} can be locally approximated by a linear space around any point x: we call these *tangent spaces*, denoted by $\mathrm{T}_x\mathrm{S}^{d-1}$. This is as opposed to a cube for which no good linearization exists at the edges. More specifically for our example, S^{d-1} is defined by the constraint $x^\top x = 1$. We may expect that differentiating this constraint should yield a suitable linearization, and indeed it does:

$$\mathrm{T}_x\mathrm{S}^{d-1} = \{v \in \mathbb{R}^d : v^\top x + x^\top v = 0\} = \{v \in \mathbb{R}^d : x^\top v = 0\}. \tag{3.3}$$

In the same spirit, it stands to reason that linear spaces and open subsets of linear spaces should also be considered smooth, as they are locally linear too.

We say a function from $\mathbb{R}^d$ to $\mathbb{R}$ is smooth if it is infinitely differentiable. We may expect that a function $f \colon \mathrm{S}^{d-1} \to \mathbb{R}$ obtained by restriction to S^{d-1} of a smooth function on $\mathbb{R}^d$ ought to be considered smooth. We adopt (essentially) this as our definition of smooth functions on S^{d-1}.

In this early chapter, we give a restricted definition of smoothness, focusing on embedded submanifolds. This allows us to build our initial toolbox more rapidly, and is sufficient to handle many applications. We extend our perspective to the general framework later on, in Chapter 8.

To get started with a list of required tools, it is useful to review briefly the main ingredients of optimization on a *linear* space $\mathcal{E}$:

$$\min_{x \in \mathcal{E}} f(x). \tag{3.4}$$

For example, $\mathcal{E} = \mathbb{R}^d$ or $\mathcal{E} = \mathbb{R}^{n \times p}$. Perhaps the most fundamental algorithm to address this class of problems is *gradient descent*, also known as *steepest descent*. Given an initial guess $x_0 \in \mathcal{E}$, this algorithm produces *iterates* on $\mathcal{E}$ (a sequence of points on $\mathcal{E}$) as follows:[1]

$$x_{k+1} = x_k - \alpha_k \mathrm{grad} f(x_k), \qquad\qquad k = 0, 1, 2, \ldots \tag{3.5}$$

where the $\alpha_k > 0$ are aptly chosen step-sizes and $\mathrm{grad} f \colon \mathcal{E} \to \mathcal{E}$ is the gradient of f. Under mild assumptions, the accumulation points of the sequence $x_0, x_1, x_2, \ldots$ have relevant properties for the optimization problem (3.4). We study these later, in Chapter 4.

From this discussion, we can identify a list of desiderata for a geometric toolbox, meant to solve

$$\min_{x \in \mathrm{S}^{d-1}} f(x) \tag{3.6}$$

with some smooth function f on the sphere. The most pressing point is to find an alternative for the implicit use of linearity in (3.5). Indeed, above, both x_k and $\mathrm{grad} f(x_k)$ are elements of $\mathcal{E}$. Since $\mathcal{E}$ is a linear space, they can be combined with linear operations. Putting aside for now the issue of defining a proper notion of gradient for a function f on S^{d-1}, we must still contend with the issue that S^{d-1} is *not* a linear space: we have no notion of linear combination here.

Alternatively, we can reinterpret iteration (3.5) and say:

> *To produce $x_{k+1} \in \mathrm{S}^{d-1}$, move away from x_k along the direction $-\mathrm{grad} f(x_k)$ over some distance, while remaining on S^{d-1}.*

Surely, if the purpose is to remain on S^{d-1}, it would make little sense to move radially away from the sphere. Rather, using the notion that smooth spaces can be linearized around x by a tangent space $\mathrm{T}_x\mathrm{S}^{d-1}$, we only consider moving along directions in $\mathrm{T}_x\mathrm{S}^{d-1}$. To this end, we introduce the concept of *retraction* at x: a map $\mathrm{R}_x \colon \mathrm{T}_x\mathrm{S}^{d-1} \to \mathrm{S}^{d-1}$ which allows us to move away from x smoothly along a prescribed tangent direction while remaining on the sphere. One suggestion might be as follows, with $\|u\| = \sqrt{u^\top u}$ (see Figure 3.1):

$$\mathrm{R}_x(v) = \frac{x + v}{\|x + v\|}. \tag{3.7}$$

In this chapter, we give definitions that allow for this natural proposal.

It remains to make sense of the notion of gradient for a function on a smooth, nonlinear space. Once more, we take inspiration from the linear case. For a smooth function $f \colon \mathcal{E} \to \mathbb{R}$, the gradient is defined with respect to an *inner*

[1] Here, x_k designates an element in a sequence $x_0, x_1, \ldots$ Sometimes, we also use subscript notation such as x_i to select the ith entry of a column vector x. Context tells which is meant.

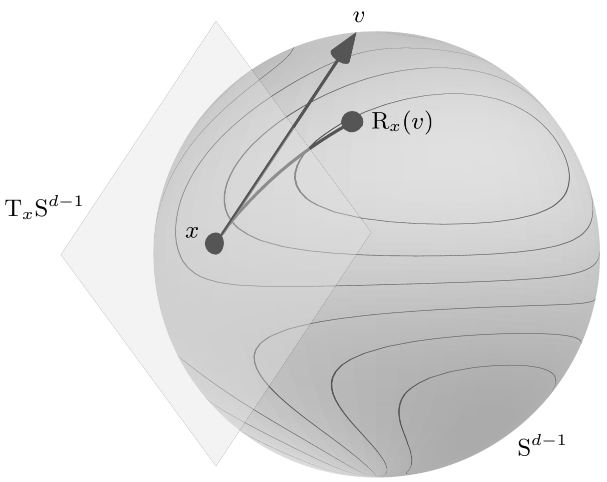


Figure 3.1 Retraction $\mathrm{R}_x(v) = \frac{x+v}{\|x+v\|}$ on the sphere.

product $\langle \cdot, \cdot \rangle : \mathcal{E} \times \mathcal{E} \to \mathbb{R}$ (see Definition 3.1 below for a reminder): $\mathrm{grad} f(x)$ is the unique element of $\mathcal{E}$ such that, for all $v \in \mathcal{E}$,

$$\mathrm{D}f(x)[v] = \langle v, \mathrm{grad} f(x) \rangle, \tag{3.8}$$

where $\mathrm{D}f(x) \colon \mathcal{E} \to \mathbb{R}$ is the differential of f at x, that is, it is the linear map defined by:

$$\mathrm{D}f(x)[v] = \lim_{t \to 0} \frac{f(x+tv) - f(x)}{t}. \tag{3.9}$$

Crucially, the gradient of f depends on a choice of inner product (while the differential of f does not).

For example, on $\mathcal{E} = \mathbb{R}^d$ equipped with the standard inner product

$$\langle u, v \rangle = u^\top v \tag{3.10}$$

and the canonical basis $e_1, \ldots, e_d \in \mathbb{R}^d$ (the columns of the identity matrix), the ith coordinate of $\mathrm{grad} f(x) \in \mathbb{R}^d$ is given by

$$\begin{aligned} \mathrm{grad} f(x)_i &= \langle e_i, \mathrm{grad} f(x) \rangle = \mathrm{D}f(x)[e_i] \\ &= \lim_{t \to 0} \frac{f(x+te_i) - f(x)}{t} \triangleq \frac{\partial f}{\partial x_i}(x), \end{aligned} \tag{3.11}$$

that is, the ith partial derivative of f as a function of $x_1, \ldots, x_d \in \mathbb{R}$. This covers a case so common that it is sometimes presented as the definition of the gradient: $\mathrm{grad} f = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \cdots & \frac{\partial f}{\partial x_d} \end{bmatrix}^\top$.

Turning to our nonlinear example again, in order to define a proper notion of gradient for $f \colon \mathrm{S}^{d-1} \to \mathbb{R}$, we find that we need to (a) provide a meaningful notion of differential $\mathrm{D}f(x) \colon \mathrm{T}_x\mathrm{S}^{d-1} \to \mathbb{R}$, and (b) introduce inner products on the tangent spaces of S^{d-1}. Let us focus on the latter for this outline.

Since $\mathrm{T}_x\mathrm{S}^{d-1}$ is a different linear subspace for various $x \in \mathrm{S}^{d-1}$, we need a different inner product for each point: $\langle \cdot, \cdot \rangle_x$ denotes our choice of inner product on $\mathrm{T}_x\mathrm{S}^{d-1}$. If this choice of inner products varies smoothly with x (in a sense we make precise below), then we call it a *Riemannian metric*, and S^{d-1} equipped with this metric is called a *Riemannian manifold.* This allows us to define the *Riemannian gradient* of f on S^{d-1}: $\mathrm{grad} f(x)$ is the unique tangent vector at x such that, for all $v \in \mathrm{T}_x\mathrm{S}^{d-1}$,

$$\mathrm{D}f(x)[v] = \langle v, \mathrm{grad} f(x) \rangle_x .$$

Thus, first we choose a Riemannian metric, then a notion of gradient ensues.

One arguably natural way of endowing S^{d-1} with a metric is to exploit the fact that each tangent space $\mathrm{T}_x\mathrm{S}^{d-1}$ is a linear subspace of $\mathbb{R}^d$, so that we may define $\langle \cdot, \cdot \rangle_x$ by restricting the inner product of $\mathbb{R}^d$ (3.10) to $\mathrm{T}_x\mathrm{S}^{d-1}$: for all $u, v \in \mathrm{T}_x\mathrm{S}^{d-1}$, $\langle u, v \rangle_x = \langle u, v \rangle$. This is indeed a Riemannian metric, and S^{d-1} endowed with this metric is called a *Riemannian submanifold* of $\mathbb{R}^d$.

For Riemannian submanifolds, the Riemannian gradient is particularly simple to compute. As per our definitions, $f \colon \mathrm{S}^{d-1} \to \mathbb{R}$ is smooth if and only if there exists a function $\bar{f} \colon \mathbb{R}^d \to \mathbb{R}$, smooth in the usual sense, such that f and $\bar{f}$ coincide on S^{d-1}. We will argue that

$$\mathrm{grad} f(x) = \mathrm{Proj}_x(\mathrm{grad} \bar{f}(x)), \qquad \text{with} \qquad \mathrm{Proj}_x(v) = (I_d - xx^\top)v,$$

where $\mathrm{Proj}_x \colon \mathbb{R}^d \to \mathrm{T}_x\mathrm{S}^{d-1}$ is the orthogonal projector from $\mathbb{R}^d$ to $\mathrm{T}_x\mathrm{S}^{d-1}$ (orthogonal with respect to the inner product on $\mathbb{R}^d$.) The functions f and $\bar{f}$ often have the same analytical expression. For example, $f(x) = x^\top Ax$ (for some matrix $A \in \mathbb{R}^{d\times d}$) is smooth on S^{d-1} because $\bar{f}(x) = x^\top Ax$ is smooth on $\mathbb{R}^d$ and they coincide on S^{d-1}. To summarize:

For Riemannian submanifolds, the Riemannian gradient is the orthogonal projection of the "classical" gradient to the tangent spaces.

With these tools in place, we can justify the following algorithm, an instance of *Riemannian gradient descent* on S^{d-1}. Given $x_0 \in \mathrm{S}^{d-1}$, let

$$\begin{aligned} x_{k+1} = \mathrm{R}_{x_k}(-\alpha_k \mathrm{grad} f(x_k)), \qquad &\text{with} \qquad \mathrm{grad} f(x) = (I_d - xx^\top)\mathrm{grad} \bar{f}(x), \\ &\text{and} \qquad \mathrm{R}_x(v) = \frac{x+v}{\|x+v\|}, \end{aligned}$$

where $\bar{f}$ is a smooth extension of f to $\mathbb{R}^d$. More importantly, these tools give us a formal framework to design and analyze such algorithms on a large class of smooth, nonlinear spaces.

We now proceed to construct precise definitions, starting with a few reminders of linear algebra and multivariate calculus in linear spaces.

3.1 Reminders of Euclidean space

The letter $\mathcal{E}$ always denotes a *linear space* (or *vector space*) over the reals, that is, a set equipped with (and closed under) vector addition and scalar multiplication by real numbers. Frequent examples include $\mathbb{R}^d$ (column vectors of length d), $\mathbb{R}^{n \times p}$ (matrices of size $n \times p$), $\mathrm{Sym}(n)$ (real, symmetric matrices of size n), $\mathrm{Skew}(n)$ (real, skew-symmetric matrices of size n), and their (linear) subspaces.

We write $\mathrm{span}(u_1, \ldots, u_m)$ to denote the subspace of $\mathcal{E}$ *spanned* by vectors $u_1, \ldots, u_m \in \mathcal{E}$. By extension, $\mathrm{span}(X)$ for a matrix $X \in \mathbb{R}^{n \times m}$ denotes the subspace of $\mathbb{R}^n$ spanned by the columns of X.

Given two linear spaces $\mathcal{E}$ and $\mathcal{F}$, a *linear map* or *linear operator* is a map $\mathcal{L} \colon \mathcal{E} \to \mathcal{F}$ such that $\mathcal{L}(au + bv) = a\mathcal{L}(u) + b\mathcal{L}(v)$ for all $u, v \in \mathcal{E}$ and $a, b \in \mathbb{R}$. We let $\operatorname{im} \mathcal{L}$ denote the *image* (or the *range*) of $\mathcal{L}$, and we let $\ker \mathcal{L}$ denote the *kernel* (or *null space*) of $\mathcal{L}$.

A *basis* for $\mathcal{E}$ is a set of vectors (elements of $\mathcal{E}$) $e_1, \ldots, e_d$ such that each vector $x \in \mathcal{E}$ can be expressed uniquely as a linear combination $x = a_1 e_1 + \cdots + a_d e_d$ with real coefficients $a_1, \ldots, a_d$. All bases have the same number of elements, called the *dimension* of $\mathcal{E}$ ($\dim \mathcal{E} = d$): it is always finite in our treatment. Each basis induces a one-to-one linear map identifying $\mathcal{E}$ and $\mathbb{R}^d$ to each other: we write $\mathcal{E} \equiv \mathbb{R}^d$.

Topology.

Recall that a *topology* on a set is a collection of subsets called *open* such that (a) the whole set and the empty set are open, (b) any union of opens is open, and (c) the intersection of a finite number of opens is open—more on this in Section 8.2. A subset is *closed* if its complement is open. A subset may be open, closed, both, or neither. We always equip $\mathbb{R}^d$ with its usual topology [Lee12, Ex. A.6]. Each linear space $\mathcal{E}$ of dimension d inherits the topology of $\mathbb{R}^d$ through their identification as above. A *neighborhood* of x in $\mathcal{E}$ is an open subset of $\mathcal{E}$ which contains x. Some authors call such sets *open* neighborhoods. All our neighborhoods are open, hence we omit the qualifier.

Euclidean structure.

It is useful to endow $\mathcal{E}$ with more structure.

Definition 3.1. *An* inner product *on $\mathcal{E}$ is a function $\langle \cdot, \cdot \rangle : \mathcal{E} \times \mathcal{E} \to \mathbb{R}$ with the following properties. For all $u, v, w \in \mathcal{E}$ and $a, b \in \mathbb{R}$, we have:*

1. *Symmetry: $\langle u, v \rangle = \langle v, u \rangle$;*
2. *Linearity: $\langle au + bv, w \rangle = a \langle u, w \rangle + b \langle v, w \rangle$; and*
3. *Positive definiteness: $\langle u, u \rangle \geq 0$ and $\langle u, u \rangle = 0 \iff u = 0$.*

Two vectors u, v are orthogonal *if $\langle u, v \rangle = 0$.*

Definition 3.2. *A linear space $\mathcal{E}$ with an inner product $\langle \cdot, \cdot \rangle$ is a* Euclidean space. *An inner product induces a norm on $\mathcal{E}$ called the* Euclidean norm*:*

$$\|u\| = \sqrt{\langle u, u \rangle}. \tag{3.12}$$

Definition 3.3. *A basis $u_1, \ldots, u_d$ of a Euclidean space $\mathcal{E}$ is* orthonormal *if*

$$\forall\, 1 \leq i, j \leq d, \qquad\qquad \langle u_i, u_j \rangle = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{otherwise.} \end{cases}$$

The standard inner product on $\mathbb{R}^d$ and the associated norm are:

$$\langle u, v \rangle = u^\top v = \sum_i u_i v_i, \qquad\qquad \|u\| = \sqrt{\sum_i u_i^2}. \tag{3.13}$$

Similarly, the standard inner product on linear spaces of matrices such as $\mathbb{R}^{n \times p}$ and $\mathrm{Sym}(n)$ is the so-called *Frobenius inner product*, with its associated *Frobenius norm*:

$$\langle U, V \rangle = \mathrm{Tr}(U^\top V) = \sum_{ij} U_{ij} V_{ij}, \qquad\qquad \|U\| = \sqrt{\sum_{ij} U_{ij}^2}, \tag{3.14}$$

where $\mathrm{Tr}(M) = \sum_i M_{ii}$ is the *trace* of a matrix. Summations are over all entries. When we do not specify it, we mean to use the standard inner product and norm.

We often use the following properties of the above inner product, with matrices U, V, W, A, B of compatible sizes:

$$\begin{aligned} \langle U, V \rangle &= \langle U^\top, V^\top \rangle, & \langle UA, V \rangle &= \langle U, VA^\top \rangle, \\ \langle BU, V \rangle &= \langle U, B^\top V \rangle, & \langle U \odot W, V \rangle &= \langle U, V \odot W \rangle, \end{aligned} \tag{3.15}$$

where $\odot$ denotes entrywise multiplication (*Hadamard product*).

Although we only consider linear spaces over the reals, we can still handle complex matrices. For example, $\mathbb{C}^n$ is a real linear space of dimension $2n$. The standard basis for it is $e_1, \ldots, e_n, ie_1, \ldots, ie_n$, where $e_1, \ldots, e_n$ form the standard basis of $\mathbb{R}^n$ (the columns of the identity matrix of size n), and i is the imaginary unit. Indeed, any vector in $\mathbb{C}^n$ can be written uniquely as a linear combination of those basis vectors using real coefficients. The standard inner product and norm on $\mathbb{C}^n$ as a real linear space are:

$$\langle u, v \rangle = \Re\{u^* v\} = \Re\left\{\sum_k \bar{u}_k v_k\right\}, \qquad\qquad \|u\| = \sqrt{\sum_k |u_k|^2}, \tag{3.16}$$

where u^* is the Hermitian conjugate-transpose of u, $\bar{u}_k$ is the complex conjugate of u_k, $|u_k|$ is its magnitude and $\Re\{a\}$ is the real part of a. This perspective is equivalent to identifying $\mathbb{C}^n$ with $\mathbb{R}^{2n}$, where real and imaginary parts are considered as two vectors in $\mathbb{R}^n$. Likewise, the set of complex matrices $\mathbb{C}^{n \times p}$ is a real linear space of dimension $2np$, with the following standard inner product and norm:

$$\langle U, V\rangle = \Re\{\mathrm{Tr}(U^*V)\} = \Re\left\{\sum_{k\ell} \bar{U}_{k\ell}V_{k\ell}\right\}, \qquad \|U\| = \sqrt{\sum_{k\ell}|U_{k\ell}|^2}. \tag{3.17}$$

The analog of (3.15) in the complex case is:

$$\begin{aligned} \langle U, V\rangle &= \langle U^*, V^*\rangle, & \langle UA, V\rangle &= \langle U, VA^*\rangle, \\ \langle BU, V\rangle &= \langle U, B^*V\rangle, & \langle U\odot W, V\rangle &= \langle U, V\odot \bar{W}\rangle. \end{aligned} \tag{3.18}$$

A linear map between two Euclidean spaces has a unique *adjoint*, which we now define. These are often useful in deriving gradients of functions—more on this in Section 4.7.

Definition 3.4. *Let $\mathcal{E}$ and $\mathcal{F}$ be two Euclidean spaces, with inner products $\langle\cdot,\cdot\rangle_{\mathcal{E}}$ and $\langle\cdot,\cdot\rangle_{\mathcal{F}}$, respectively. Let $\mathcal{L}\colon \mathcal{E}\to\mathcal{F}$ be a linear map. The* adjoint *of $\mathcal{L}$ is the linear map $\mathcal{L}^*\colon \mathcal{F}\to\mathcal{E}$ defined by the following property:*

$$\forall u\in\mathcal{E}, v\in\mathcal{F}, \qquad \langle \mathcal{L}(u), v\rangle_{\mathcal{F}} = \langle u, \mathcal{L}^*(v)\rangle_{\mathcal{E}}\,.$$

Definition 3.5. *Let $\mathcal{E}$ be a Euclidean space with inner product $\langle\cdot,\cdot\rangle$. If the linear map $\mathcal{A}\colon\mathcal{E}\to\mathcal{E}$ satisfies*

$$\forall u, v\in\mathcal{E}, \qquad \langle\mathcal{A}(u), v\rangle = \langle u, \mathcal{A}(v)\rangle\,,$$

that is, if $\mathcal{A} = \mathcal{A}^*$, we say $\mathcal{A}$ is self-adjoint *or* symmetric*.*

As we can see from (3.15) and (3.18), adjoints and matrix transposes are intimately related: it is an exercise to make this precise.

Self-adjoint linear maps have important spectral properties.

Theorem 3.6 (Spectral theorem)**.** *A self-adjoint map $\mathcal{A}$ on a Euclidean space $\mathcal{E}$ admits an orthonormal basis of eigenvectors $v_1,\ldots,v_d\in\mathcal{E}$ associated to real eigenvalues $\lambda_1,\ldots,\lambda_d$ so that $\mathcal{A}(v_i) = \lambda_i v_i$ for $i = 1,\ldots,d$ with $d = \dim\mathcal{E}$.*

Definition 3.7. *A self-adjoint map $\mathcal{A}$ on $\mathcal{E}$ is* positive semidefinite *if, for all $u\in\mathcal{E}$, we have $\langle u,\mathcal{A}(u)\rangle\geq 0$; we write $\mathcal{A}\succeq 0$. Owing to the spectral theorem, this is equivalent to all eigenvalues of $\mathcal{A}$ being nonnegative. Similarly, $\mathcal{A}$ is* positive definite *if $\langle u,\mathcal{A}(u)\rangle > 0$ for all nonzero $u\in\mathcal{E}$; we write $\mathcal{A}\succ 0$. This is equivalent to all eigenvalues of $\mathcal{A}$ being positive.*

Norms on vector spaces induce norms for linear maps.

Definition 3.8. *The* operator norm *of $\mathcal{L}\colon\mathcal{E}\to\mathcal{F}$ is defined as*

$$\|\mathcal{L}\| = \max_{u\in\mathcal{E}, u\neq 0}\frac{\|\mathcal{L}(u)\|_{\mathcal{F}}}{\|u\|_{\mathcal{E}}},$$

where $\|\cdot\|_{\mathcal{E}}$ and $\|\cdot\|_{\mathcal{F}}$ denote the norms on the Euclidean spaces $\mathcal{E}$ and $\mathcal{F}$, respectively.

Equivalently, $\|\mathcal{L}\|$ is the smallest real such that $\|\mathcal{L}(u)\|_{\mathcal{F}} \leq \|\mathcal{L}\|\|u\|_{\mathcal{E}}$ for all u in $\mathcal{E}$. The *singular values* of $\mathcal{L}$ are the nonnegative square roots of the eigenvalues of $\mathcal{L}^* \circ \mathcal{L}$, and $\|\mathcal{L}\|$ is the largest singular value of $\mathcal{L}$. For a self-adjoint map $\mathcal{A}$ with eigenvalues $\lambda_1, \ldots, \lambda_d$, it follows that $\|\mathcal{A}\| = \max_{1 \leq i \leq d} |\lambda_i|$.

Calculus.

We write $F \colon A \to B$ to designate a map F whose domain is all of A. If C is a subset of A, we write $F|_C \colon C \to B$ to designate the *restriction* of F to the domain C, so that $F|_C(x) = F(x)$ for all $x \in C$.

Let U, V be open sets in two linear spaces $\mathcal{E}, \mathcal{F}$. A map $F \colon U \to V$ is *smooth* if it is infinitely differentiable (class C^∞) on its domain. We also say that F is *smooth at a point* $x \in U$ if there exists a neighborhood U' of x such that $F|_{U'}$ is smooth. Accordingly, F is smooth if it is smooth at all points in its domain.

If $F \colon U \to V$ is smooth at x, the *differential* of F at x is the linear map $\mathrm{D}F(x) \colon \mathcal{E} \to \mathcal{F}$ defined by

$$\mathrm{D}F(x)[u] = \frac{\mathrm{d}}{\mathrm{d}t} F(x + tu)\bigg|_{t=0} = \lim_{t \to 0} \frac{F(x + tu) - F(x)}{t}. \tag{3.19}$$

For a curve $c \colon \mathbb{R} \to \mathcal{E}$, we write c' to denote its velocity: $c'(t) = \frac{\mathrm{d}}{\mathrm{d}t} c(t)$.

For a smooth function $f \colon \mathcal{E} \to \mathbb{R}$ defined on a Euclidean space $\mathcal{E}$, the (Euclidean) *gradient* of f is the map $\mathrm{grad} f \colon \mathcal{E} \to \mathcal{E}$ defined by the following property:

$$\forall x, v \in \mathcal{E}, \qquad \langle \mathrm{grad} f(x), v \rangle = \mathrm{D}f(x)[v].$$

The (Euclidean) *Hessian* of f at x is the linear map $\mathrm{Hess} f(x) \colon \mathcal{E} \to \mathcal{E}$ defined by

$$\mathrm{Hess} f(x)[v] = \mathrm{D}(\mathrm{grad} f)(x)[v] = \lim_{t \to 0} \frac{\mathrm{grad} f(x + tv) - \mathrm{grad} f(x)}{t}.$$

The *Clairaut–Schwarz theorem* implies that $\mathrm{Hess} f(x)$ is self-adjoint with respect to the inner product of $\mathcal{E}$.

Exercise 3.9 (Adjoint and transpose)**.** *Let $u_1, \ldots, u_n$ form an orthonormal basis of $\mathcal{E}$. Likewise, let $v_1, \ldots, v_m$ form an orthonormal basis of $\mathcal{F}$. Consider a linear map $\mathcal{L} \colon \mathcal{E} \to \mathcal{F}$. For each $1 \leq i \leq n$, the vector $\mathcal{L}(u_i)$ is an element of $\mathcal{F}$; therefore, it expands uniquely in the basis $v_1, \ldots, v_m$ as follows:*

$$\mathcal{L}(u_i) = \sum_{j=1}^{m} M_{ji} v_j,$$

where we collect the coefficients into a matrix $M \in \mathbb{R}^{m \times n}$. This matrix represents *$\mathcal{L}$ with respect to the chosen bases. Show that the matrix which represents $\mathcal{L}^*$ with respect to those same bases is $M^\top$: the transpose of M. In particular, a linear map $\mathcal{A} \colon \mathcal{E} \to \mathcal{E}$ is self-adjoint if and only if the matrix associated to it with respect to the basis $u_1, \ldots, u_n$ is symmetric.*

3.2 Embedded submanifolds of a linear space

We set out to define what it means for a subset $\mathcal{M}$ of a linear space $\mathcal{E}$ to be smooth. Our main angle is to capture the idea that a smooth set can be linearized in some meaningful way around each point. To make sense of what that might mean, consider the sphere S^{d-1}. This is the set of vectors $x \in \mathbb{R}^d$ satisfying

$$h(x) = x^\top x - 1 = 0.$$

As we discussed in the introduction, it can be adequately linearized around each point by the set (3.3). The perspective we used to obtain this linearization is that of differentiating the defining equation. More precisely, consider a truncated Taylor expansion of h:

$$h(x + tv) = h(x) + t\,\mathrm{D}h(x)[v] + O(t^2).$$

If x is in S^{d-1} and v is in $\ker \mathrm{D}h(x)$ (so that $h(x) = 0$ and $\mathrm{D}h(x)[v] = 0$), then $h(x + tv) = O(t^2)$, indicating that $x + tv$ nearly satisfies the defining equation of S^{d-1} for small t. This motivates us to consider the subspace $\ker \mathrm{D}h(x)$ as a linearization of S^{d-1} around x. Since

$$\mathrm{D}h(x)[v] = \lim_{t \to 0} \frac{h(x + tv) - h(x)}{t} = x^\top v + v^\top x = 2x^\top v,$$

the kernel of $\mathrm{D}h(x)$ is the subspace orthogonal to x in $\mathbb{R}^d$ (with respect to the usual inner product). This coincides with (3.3), arguably in line with intuition.

At first, one might think that if a set is defined by an equation of the form $h(x) = 0$ with some smooth function h, then that set is smooth and can be linearized by the kernels of $\mathrm{D}h$. However, this is not the case. Indeed, consider the following example in $\mathbb{R}^2$ (see Figure 3.2):

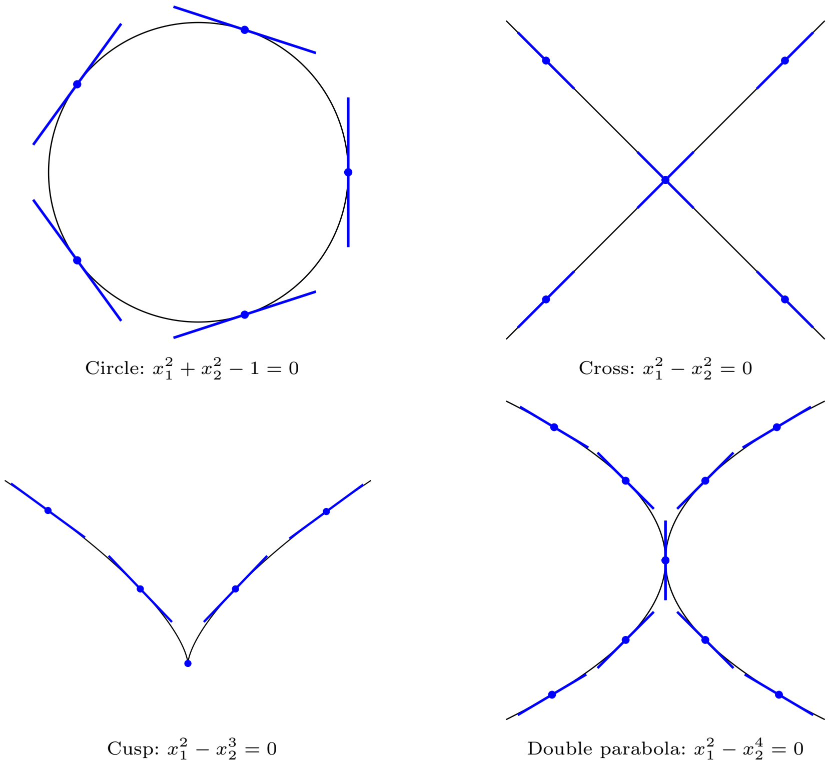
$$\mathcal{X} = \left\{x \in \mathbb{R}^2 : h(x) = x_1^2 - x_2^2 = 0\right\}.$$

The defining function h is smooth, yet the set $\mathcal{X}$ is a cross in the plane formed by the union of the lines $x_1 = x_2$ and $x_1 = -x_2$. We want to exclude such sets because of the kink at the origin. What went wrong with it? If we blindly use the kernel of the differential to linearize $\mathcal{X}$, we first determine

$$\mathrm{D}h(x) = \left[\frac{\partial h}{\partial x_1}(x), \frac{\partial h}{\partial x_2}(x)\right] = [2x_1, -2x_2].$$

At $x = 0$, $\mathrm{D}h(0) = [0, 0]$, whose kernel is all of $\mathbb{R}^2$: that does not constitute a reasonable linearization of $\mathcal{X}$ around the origin.

We can gain further insight into the issue at hand by considering additional examples. The zero-sets of the functions $h(x) = x_1^2 - x_2^3$ and $h(x) = x_1^2 - x_2^4$ from $\mathbb{R}^2$ to $\mathbb{R}$, respectively, define a cusp and a double parabola, both of which fail our intuitive test of smoothness at the origin. What the cross, cusp and double parabola have in common is that the rank of $\mathrm{D}h(x)$ suddenly drops from one to zero at the origin, whereas for the sphere that rank is constant (and maximal) on the whole set.



Circle: $x_1^2 + x_2^2 - 1 = 0$

Cross: $x_1^2 - x_2^2 = 0$

Cusp: $x_1^2 - x_2^3 = 0$

Double parabola: $x_1^2 - x_2^4 = 0$

Figure 3.2 Four different sets $\mathcal{S}$ defined as the zero-sets of a smooth function from $\mathbb{R}^2$ to $\mathbb{R}$. For each, the sets $\mathrm{T}_x\mathcal{S}$ (Definition 3.14) are drawn at a few different points. Only the circle (top left) is an embedded submanifold of $\mathbb{R}^2$.

These observations motivate the definition below. Since smoothness is a local notion, the definition is phrased in terms of what the set $\mathcal{M}$ looks like around each point. Since a set $\mathcal{M}$ may be equivalently defined by many different functions h, and since it may not be practical (or even possible, see Section 3.10) to define all of $\mathcal{M}$ with a single function h, the definition allows for a different one to be used around each point.

Definition 3.10. *Let $\mathcal{E}$ be a linear space of dimension d. A non-empty subset $\mathcal{M}$ of $\mathcal{E}$ is a* (smooth) embedded submanifold of $\mathcal{E}$ of dimension n *if either*

1. *$n = d$ and $\mathcal{M}$ is open in $\mathcal{E}$—we also call this an* open submanifold*; or*
2. *$n = d - k$ for some $k \geq 1$ and, for each $x \in \mathcal{M}$, there exists a neighborhood U of x in $\mathcal{E}$ and a smooth function $h \colon U \to \mathbb{R}^k$ such that*
   (a) If y is in U, then $h(y) = 0$ if and only if $y \in \mathcal{M}$; and
   (b) $\operatorname{rank} \mathrm{D}h(x) = k$.
   Such a function h is called a local defining function *for $\mathcal{M}$ at x.*

If $\mathcal{M}$ is a linear (sub)space, we also call it a linear manifold.

Condition 2(a) in the previous definition can be stated equivalently as:

$$\mathcal{M} \cap U = h^{-1}(0) \triangleq \{y \in U : h(y) = 0\}.$$

It is an exercise to verify that Definition 3.10 excludes various pathological sets such as the cross ($x_1^2 = x_2^2$), cusp ($x_1^2 = x_2^3$) and double parabola ($x_1^2 = x_2^4$).

Differential geometry defines a broader class of smooth sets called *(smooth) manifolds*. We typically omit the word 'smooth' as all of our manifolds are smooth, though bear in mind that in the literature there exist different kinds of manifolds, not all of which are smooth. Embedded submanifolds are manifolds. When the statements we make hold true for smooth manifolds in general, we use the word manifold (rather than embedded submanifold) to signal it. This is common throughout Chapters 3 and 5. ⋆

The hope is that limiting our initial treatment of manifolds to embedded submanifolds provides a more intuitive entry point to build all the tools we need for optimization. This is all the more relevant considering that many of the manifolds we encounter in applications are in fact embedded submanifolds, presented to us as zero-sets of their local defining functions. All of our optimization algorithms work on general manifolds. The general theory is in Chapter 8.

To build additional support for our definition of embedded submanifolds, we further argue that small patches of $\mathcal{M}$ can be deformed into linear subspaces in a smooth and smoothly invertible way. This captures an important feature of smoothness, namely: upon zooming close to a point of $\mathcal{M}$, what we see can hardly be distinguished from what we would have seen had $\mathcal{M}$ been a linear subspace of $\mathcal{E}$.

Definition 3.11. *A* diffeomorphism *is a bijective map $F \colon U \to V$, where U, V are open sets and such that both F and F^{-1} are smooth.*

Theorem 3.12. *Let $\mathcal{E}$ be a linear space of dimension d. A subset $\mathcal{M}$ of $\mathcal{E}$ is an embedded submanifold of $\mathcal{E}$ of dimension $n = d - k$ if and only if for each $x \in \mathcal{M}$ there exists a neighborhood U of x in $\mathcal{E}$, an open set V in $\mathbb{R}^d$ and a diffeomorphism $F \colon U \to V$ such that $F(\mathcal{M} \cap U) = E \cap V$, where $E = \{y \in \mathbb{R}^d : y_{n+1} = \cdots = y_d = 0\}$ is a linear subspace of $\mathbb{R}^d$.*

The main tool we need to prove Theorem 3.12 is the standard *inverse function theorem*, stated here without proof [Lee12, Thm. C.34].

Theorem 3.13 (Inverse function theorem)**.** *Suppose $U \subseteq \mathcal{E}$ and $V \subseteq \mathcal{F}$ are open subsets of linear spaces of the same dimension, and $F \colon U \to V$ is smooth. If $\mathrm{D}F(x)$ is invertible at some point $x \in U$, then there exist neighborhoods $U' \subseteq U$ of x and $V' \subseteq V$ of $F(x)$ such that $F|_{U'} \colon U' \to V'$ (the restriction of F to U' and V') is a diffeomorphism.*

Equipped with this tool, we proceed to prove Theorem 3.12.

Proof of Theorem 3.12. We prove one direction of the theorem, namely: we assume $\mathcal{M}$ is an embedded submanifold and construct diffeomorphisms F. The other direction is left as an exercise. For the latter, it is helpful to note that if F is a diffeomorphism with inverse F^{-1}, then $\mathrm{D}F(x)$ is invertible and

$$(\mathrm{D}F(x))^{-1} = \mathrm{D}F^{-1}(F(x)). \tag{3.20}$$

To see this, apply the chain rule to differentiate $F^{-1} \circ F$, noting that this is nothing but the identity map.

If $n = d$ (that is, $\mathcal{M}$ is open in $\mathcal{E}$), the claim is clear: simply let F be any invertible linear map from $\mathcal{E}$ to $\mathbb{R}^d$ (for example, using a basis of $\mathcal{E}$), and restrict its domain and codomain to $U = \mathcal{M}$ and $V = F(U)$.

We now consider the more interesting case where $n = d - k$ with $k \geq 1$. Let $h \colon U \to \mathbb{R}^k$ be any local defining function for $\mathcal{M}$ at x. We work in coordinates on $\mathcal{E}$, which is thus identified with $\mathbb{R}^d$. Then, we can think of $\mathrm{D}h(x)$ as a matrix of size $k \times d$. By assumption, $\mathrm{D}h(x)$ has rank k. This means that it is possible to pick k columns of that matrix which form a $k \times k$ invertible matrix. If needed, permute the chosen coordinates so that the last k columns have that property (this is without loss of generality). Then, we can write $\mathrm{D}h(x)$ in block form so that

$$\mathrm{D}h(x) = \begin{bmatrix} A & B \end{bmatrix},$$

where $B \in \mathbb{R}^{k \times k}$ is invertible and A is in $\mathbb{R}^{k \times (d-k)}$. Now consider the function $F \colon U \to \mathbb{R}^d$ (recall $U \subseteq \mathcal{E}$ is the domain of h) defined by

$$F(y) = (y_1, \ldots, y_{d-k}, h_1(y), \ldots, h_k(y))^\top, \tag{3.21}$$

where $y_1, \ldots, y_d$ denote the coordinates of $y \in \mathcal{E}$. In order to apply the inverse function theorem to F at x, we must verify that F is smooth—this is clear—and that the differential of F at x is invertible. Working this out one row at a time, we get the following expression for that differential:

$$\mathrm{D}F(x) = \begin{bmatrix} I_{d-k} & 0 \\ A & B \end{bmatrix},$$

where I_{d-k} is the identity matrix of size $d-k$, and 0 here denotes a zero matrix of size $(d-k) \times k$. The matrix $\mathrm{D}F(x)$ is invertible, as demonstrated by the following expression for its inverse:

$$(\mathrm{D}F(x))^{-1} = \begin{bmatrix} I_{d-k} & 0 \\ -B^{-1}A & B^{-1} \end{bmatrix}. \tag{3.22}$$

(Indeed, their product is I_d.) Hence, the inverse function theorem asserts that we may reduce U to a possibly smaller neighborhood of x so that F (now restricted to that new neighborhood) is a diffeomorphism from U to $V = F(U)$. The property $F(\mathcal{M} \cap U) = E \cap V$ follows by construction of F from the property $\mathcal{M} \cap U = h^{-1}(0)$. □

In order to understand the local geometry of a set around a point, we aim to describe acceptable directions of movement through that point. This is close in spirit to the tools we look to develop for optimization, as they involve moving away from a point while remaining on the set. Specifically, for a subset $\mathcal{M}$ of a linear space $\mathcal{E}$, consider all the smooth curves of $\mathcal{E}$ which lie entirely on $\mathcal{M}$ and pass through a given point x. Collect their velocities as they do so in a set $\mathrm{T}_x\mathcal{M}$ defined below. In that definition, c is smooth in the usual sense as a map from (an open subset of) $\mathbb{R}$ to $\mathcal{E}$—two linear spaces.

Definition 3.14. *Let $\mathcal{M}$ be a subset of $\mathcal{E}$. For all $x \in \mathcal{M}$, define:*

$$\mathrm{T}_x\mathcal{M} = \{c'(0) \mid c\colon I \to \mathcal{M} \text{ is smooth and } c(0) = x\}, \tag{3.23}$$

where I is any open interval containing $t = 0$. That is, v is in $\mathrm{T}_x\mathcal{M}$ if and only if there exists a smooth curve on $\mathcal{M}$ passing through x with velocity v.

Note that $\mathrm{T}_x\mathcal{M}$ is a subset of $\mathcal{E}$. For the sphere, it is easy to convince oneself that $\mathrm{T}_x\mathcal{M}$ coincides with the subspace in (3.3). We show in the next theorem that this is always the case for embedded submanifolds.

Theorem 3.15. *Let $\mathcal{M}$ be an embedded submanifold of $\mathcal{E}$. Consider $x \in \mathcal{M}$ and the set $\mathrm{T}_x\mathcal{M}$ (3.23). If $\mathcal{M}$ is an open submanifold, then $\mathrm{T}_x\mathcal{M} = \mathcal{E}$. Otherwise, $\mathrm{T}_x\mathcal{M} = \ker \mathrm{D}h(x)$ with h any local defining function at x.*

Proof. For open submanifolds, the claim is clear. By definition, $\mathrm{T}_x\mathcal{M}$ is included in $\mathcal{E}$. The other way around, for any $v \in \mathcal{E}$, consider $c(t) = x + tv$: this is a smooth curve from some non-empty interval around 0 to $\mathcal{M}$ such that $c(0) = x$, hence $v = c'(0)$ is in $\mathrm{T}_x\mathcal{M}$. This shows $\mathcal{E}$ is included in $\mathrm{T}_x\mathcal{M}$, so that the two coincide.

Now consider the case of $\mathcal{M}$ an embedded submanifold of dimension $n = d - k$ with $k \geq 1$. Let $h\colon U \to \mathbb{R}^k$ be a local defining function of $\mathcal{M}$ around x. The proof is in two steps. First, we show that $\mathrm{T}_x\mathcal{M}$ is included in $\ker \mathrm{D}h(x)$. Then, we show that $\mathrm{T}_x\mathcal{M}$ contains a linear subspace of the same dimension as $\ker \mathrm{D}h(x)$. These two facts combined indeed confirm that $\mathrm{T}_x\mathcal{M} = \ker \mathrm{D}h(x)$.

Step 1. If v is in $\mathrm{T}_x\mathcal{M}$, there exists $c\colon I \to \mathcal{M}$, smooth, such that $c(0) = x$ and $c'(0) = v$. Since $c(t)$ is in $\mathcal{M}$, we have $h(c(t)) = 0$ for all $t \in I$ (if need be, restrict the interval I to ensure $c(t)$ remains in the domain of h). Thus, the derivative of $h \circ c$ vanishes at all times:

$$0 = \frac{\mathrm{d}}{\mathrm{d}t} h(c(t)) = \mathrm{D}h(c(t))[c'(t)].$$

In particular, at $t = 0$ this implies $\mathrm{D}h(x)[v] = 0$, that is, $v \in \ker \mathrm{D}h(x)$. This confirms $\mathrm{T}_x\mathcal{M} \subseteq \ker \mathrm{D}h(x)$.

Step 2. To show that $\mathrm{T}_x\mathcal{M}$ contains a subspace of the same dimension as $\ker \mathrm{D}h(x)$ (namely, of dimension $n = d - k$), we must construct smooth curves on $\mathcal{M}$ that pass through x with various velocities. To do so, we call upon Theorem 3.12. The latter provides us with a diffeomorphism $F\colon U \to V$ (where U is now a possibly smaller neighborhood of x than the original domain of h.) We use F^{-1} to construct smooth curves on $\mathcal{M}$ that pass through x. Specifically, pick an arbitrary $u \in \mathbb{R}^{d-k}$ and let

$$\gamma(t) = F(x) + t \begin{bmatrix} u \\ 0 \end{bmatrix}.$$

(Here, 0 denotes a zero vector of size k.) Notice that γ remains in $E \cap V$ for t close to zero, where E is the subspace of $\mathbb{R}^d$ consisting of all vectors whose last k entries are zero. Since $F^{-1}(E \cap V) = \mathcal{M} \cap U$, it follows that

$$c(t) = F^{-1}(\gamma(t)) \tag{3.24}$$

resides in $\mathcal{M}$ for t close to zero. Moreover, $c(0) = x$ and c is smooth since F^{-1} is smooth. It follows that c is indeed a smooth curve on $\mathcal{M}$ passing through x. What is the velocity of this curve at x? Applying the chain rule to (3.24), we get

$$c'(t) = \mathrm{D}F^{-1}(\gamma(t))\,[\gamma'(t)].$$

In particular, at $t = 0$ we have

$$c'(0) = \mathrm{D}F^{-1}(F(x)) \begin{bmatrix} u \\ 0 \end{bmatrix}.$$

Since F is a diffeomorphism, we know from (3.20) that $\mathrm{D}F^{-1}(F(x))$ is an invertible linear map, equal to $(\mathrm{D}F(x))^{-1}$. The specific form of $c'(0)$ is unimportant. What matters is that each $c'(0)$ of the form above certainly belongs to $\mathrm{T}_x\mathcal{M}$ (3.23). Since $\mathrm{D}F^{-1}(F(x))$ is invertible and $u \in \mathbb{R}^{d-k}$ is arbitrary, this means that $\mathrm{T}_x\mathcal{M}$ contains a subspace of dimension $d-k$. But we know from the previous step that $\mathrm{T}_x\mathcal{M}$ is included in a subspace of dimension $d-k$, namely, $\ker \mathrm{D}h(x)$. It follows that $\mathrm{T}_x\mathcal{M} = \ker \mathrm{D}h(x)$. Since this holds for all $x \in \mathcal{M}$, the proof is complete. □

Thus, for an embedded submanifold $\mathcal{M}$ of dimension $n = d - k$, for each x in $\mathcal{M}$, the set $\mathrm{T}_x\mathcal{M}$ is a linear subspace of $\mathcal{E}$ of dimension n. These subspaces are the linearizations of the smooth set $\mathcal{M}$.

Definition 3.16. *We call* $\mathrm{T}_x\mathcal{M}$ *the* tangent space *to* $\mathcal{M}$ *at* x*. Vectors in* $\mathrm{T}_x\mathcal{M}$ *are called* tangent vectors *to* $\mathcal{M}$ *at* x*. The dimension of* $\mathrm{T}_x\mathcal{M}$ *(which is independent of* x*) coincides with the* dimension of $\mathcal{M}$*, denoted by* $\dim \mathcal{M}$*.*

We consider three brief examples of embedded submanifolds: two obvious by now, and one arguably less obvious. It is good to keep all three in mind when assessing whether a certain proposition concerning embedded submanifolds is likely to be true. Chapter 7 details further examples.

Example 3.17. *The set* $\mathbb{R}^d$ *is a linear manifold of dimension* d *with tangent spaces* $\mathrm{T}_x\mathcal{M} = \mathbb{R}^d$ *for all* $x \in \mathbb{R}^d$*. The affine space* $\{x \in \mathbb{R}^d : Ax = b\}$ *defined by a matrix* $A \in \mathbb{R}^{k \times d}$ *of rank* k *and arbitrary vector* $b \in \mathbb{R}^k$ *is a manifold of dimension* $n = d - k$ *embedded in* $\mathbb{R}^d$*.*