

Appendix A

Notation

This is a brief guide to the notational conventions used in this text.

Scalars, vectors and matrices

We denote scalars by either small or capital letters a, A, α . We denote column vectors by bold small letters \mathbf{a}, ϕ . When we need a row vector we usually present this as the transpose of a column vector \mathbf{a}^T, ϕ^T .

We represent matrices by bold capital letters \mathbf{B}, Φ . The i^{th} row and j^{th} column of matrix \mathbf{A} is written as a_{ij} . The j^{th} column of matrix \mathbf{A} is written as \mathbf{a}_j . When we need to refer to the i^{th} row of a matrix, we write this as $\mathbf{a}_{i\bullet}$ where the bullet \bullet indicates that we are considering all possible values of the column index.

We concatenate two $D \times 1$ column vectors horizontally as $\mathbf{a} = [\mathbf{b}, \mathbf{c}]$ to form the $D \times 2$ matrix \mathbf{A} . We concatenate two $D \times 1$ column vectors vertically as $\mathbf{a} = [\mathbf{b}^T, \mathbf{c}^T]^T$ to form the $2D \times 1$ vector \mathbf{a} . Although this notation is cumbersome, it allows us to represent vertical concatenations within a single line of text.

Variables and parameters

We denote variables with Roman letters \mathbf{a}, \mathbf{b} . The most common examples are the observed data which is always denoted by \mathbf{x} and the state of the world which is always denoted by \mathbf{w} . However, other hidden or latent variables are also represented by Roman letters. We denote parameters of the model by Greek letters μ, Φ, σ^2 . These are distinguished from variables in that there is usually a single set of parameters that explains the relation between many sets of variables.

Functions

We write functions as a name, followed by square brackets that contain the arguments of the function. For example, $\log[x]$ returns the logarithm of the scalar variable x . Sometimes we will write a function with bullets \bullet as arguments (e.g., $\text{atan2}[\bullet, \bullet]$) to focus the interest on the function itself rather than the arguments.

When the function returns one or more vector or matrix arguments, it is written in bold. For example, the function $\mathbf{aff}[\mathbf{x}, \Phi, \tau]$ applies an affine transformation to the 2D point \mathbf{x} with parameters Φ, τ and returns a new 2D vector output. When a

function returns multiple outputs, we write this in Matlab notation so $[\mathbf{U}, \mathbf{L}, \mathbf{V}] = \text{svd}[\mathbf{X}]$ returns the three parts $\mathbf{U}, \mathbf{L}, \mathbf{V}$ of the singular value decomposition of \mathbf{X} .

Some functions are used repeatedly throughout the text. These include:

- $\min_x f[x]$, which returns the minimum possible value of the function $f[x]$ as we vary x over its entire valid range,
- $\text{argmin}_x f[x]$, which returns the value of the argument x that minimizes $f[x]$,
- \max_x and argmax_x , which fulfill the same roles as \min_x and argmin_x but where we are maximizing the function,
- $\text{diag}[\mathbf{A}]$, which returns a column vector containing the elements on the diagonal of matrix \mathbf{A} ,
- $\delta[x]$ for continuous x , which is a Dirac delta function and has the key property $\int f[x]\delta[x - x_0]dx = f[x_0]$,
- $\delta[x]$ for discrete x , which returns 1 when the argument x is 0 and returns 0 otherwise, and
- $\text{heaviside}[x]$, which represents the Heaviside step function. It returns 0 when the argument $x < 0$ and returns 1 otherwise.

Probability distributions

We write the probability of a random variable x as $Pr(x)$. We write the joint probability of two variables a, b as $Pr(a, b)$ and the conditional probability of a given b as $Pr(a|b)$. Sometimes, we wish to specify the exact value b^* that a is conditioned upon and here we write $Pr(a|b = b^*)$. Occasionally, we denote that variables a and b are independent by writing $a \perp\!\!\!\perp b$. Similarly we indicate that a and b are conditionally independent given c by writing $a \perp\!\!\!\perp b|c$.

Probability distributions are written in the style $Pr(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \text{Norm}_{\mathbf{x}}[\boldsymbol{\mu}, \boldsymbol{\Sigma}]$. This returns the value of the multivariate normal distribution for data \mathbf{x} when the distribution has mean $\boldsymbol{\mu}$ and covariance $\boldsymbol{\Sigma}$. In this way, we always distinguish the argument of the distribution (here \mathbf{x}) from the parameters (here $\boldsymbol{\mu}, \boldsymbol{\Sigma}$).

Sets

We denote sets with calligraphic letters \mathcal{S} . The notation $\mathcal{S} \subset \mathcal{T}$ indicates that \mathcal{S} is a subset of \mathcal{T} . The notation $x \in \mathcal{S}$ indicates that x is a member of the set \mathcal{S} . The notation $\mathcal{A} = \mathcal{B} \cup \mathcal{C}$ indicates that set \mathcal{A} is the union of sets \mathcal{B} and \mathcal{C} . The notation $\mathcal{A} = \mathcal{B} \setminus \mathcal{C}$ indicates that set \mathcal{A} consists of all of the elements of \mathcal{B} except those that are in \mathcal{C} .

Often we write out a set explicitly in terms of the elements and for this we use curly brackets so that $\mathcal{A} = \{x, y, z\}$ indicates that the set \mathcal{A} contains x , y , and z and nothing else. When a set is empty, we write $\mathcal{A} = \{\}$. We use the notation $\{x_i\}_{i=1}^I$ as shorthand to represent the set $\{x_1, x_2, \dots, x_I\}$, and we may write the same set in the compact form $x_{1..I}$ if it is part of an equation.

Appendix B

Optimization

Throughout this book, we have used iterative nonlinear optimization methods to find the maximum likelihood or MAP parameter estimates. We now provide more details about these methods. It is impossible to do full justice to this topic in the space available; many entire books have been written about nonlinear optimization. Our goal is merely to provide a brief introduction to the main ideas.

B.1 Problem statement

Continuous nonlinear optimization techniques aim to find the set of parameters $\hat{\theta}$ that minimize a function $f[\bullet]$. In other words, they try to compute,

$$\hat{\theta} = \underset{\theta}{\operatorname{argmin}} [f[\theta]], \quad (\text{B.1})$$

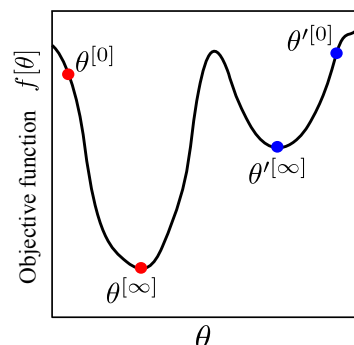
where $f[\bullet]$ is termed a *cost function* or *objective function*.

Although optimization techniques are usually described in terms of minimizing a function, most optimization problems in this book involve *maximizing* an objective function based on log probability. To turn a maximization problem into a minimization we multiply the objective function by minus one. In other words, instead of maximizing the log probability, we minimize the negative log probability.

B.1.1 Convexity

The optimization techniques that we consider here are iterative: they start with an estimate $\theta^{[0]}$ and improve it by finding successive new estimates $\theta^{[1]}, \theta^{[2]}, \dots, \theta^{[\infty]}$, each of which is better than the last, until no more improvement can be made. The techniques are purely local in the sense that the decision about where to move next is based on only the properties of the function at the current position. Consequently, these techniques cannot guarantee the correct solution: they may find an estimate $\theta^{[\infty]}$ from which no local change improves the cost. However, this

Figure B.1 Local minima. Optimization methods aim to find the minimum of the objective function $f[\theta]$ with respect to parameters θ . Roughly, they work by starting with an initial estimate $\theta^{[0]}$ and moving iteratively downhill until no more progress can be made (final position represented by $\theta^{[\infty]}$). Unfortunately, it is possible to terminate in a local minimum. For example, if we start at $\theta'^{[0]}$ and move downhill, we wind up in position $\theta'^{[\infty]}$.



does not mean there is not a better solution in some distant part of the function that has not yet been explored (figure B.1). In optimization parlance, they can only find *local minima*. One way to mitigate this problem is to start the optimization from a number of different places and choose the final solution with the lowest cost.

In the special case where the function is *convex*, there will only be a single minimum, and we are guaranteed to find it with sufficient iterations (figure B.2). For a 1D function, it is possible to establish the convexity by looking at the second derivative of the function; if this is positive everywhere (i.e., the slope is continuously increasing) then the function is convex and the global minimum can be found. The equivalent test in higher dimensions is to examine the *Hessian matrix* (the matrix of second derivatives of the cost function with respect to the parameters). If this is positive definite everywhere (see appendix C.2.6), then the function is convex and the global minimum will be found. Some of the cost functions in this book are convex, but this is unusual; most optimization problems found in vision do not have this convenient property.

B.1.2 Overview of approach

In general the parameters θ over which we search are multidimensional. For example, when θ has two dimensions, we can think of the function as a two dimensional surface (figure B.3). With this in mind, the principles behind the methods we will discuss are simple. We alternately

- choose a search direction \mathbf{s} based on the local properties of the function, and
- search to find the minimum along the chosen direction. In other words, we seek the distance λ to move such that

$$\hat{\lambda} = \underset{\lambda}{\operatorname{argmin}} \left[f[\theta^{[t]} + \lambda \mathbf{s}] \right], \quad (\text{B.2})$$

and then set $\theta^{[t+1]} = \theta^{[t]} + \hat{\lambda} \mathbf{s}$. This is termed a *line search*.

We now consider each of these stages in turn.

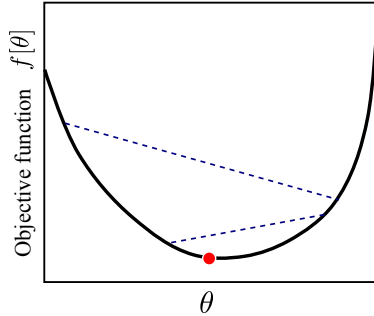


Figure B.2 Convex functions. If the function is convex, then the global minimum can be found. A function is convex if no chord (line between two points on the function) intersects the function. The figure shows two example chords (blue dashed lines). The convexity of a function can be established algebraically by considering the matrix of second derivatives. If this is positive definite for all values of θ , then the function is convex.

B.2 Choosing a search direction

We will describe two general methods for choosing a search direction (*steepest descent* and *Newton's method*) and one method which is specialized for least squares problems (the *Gauss-Newton method*). All of these methods rely on computing derivatives of the function with respect to the parameters at the current position. To this end, we are relying on the function being smooth so that the derivatives are well behaved.

For most models, it is easy to find a closed form expression for the derivatives. If this is not the case, then an alternative is to approximate them using finite differences. For example, the first derivative of $f[\bullet]$ with respect to the j^{th} element of θ can be approximated by

$$\frac{\partial f}{\partial \theta_j} \approx \frac{f[\theta + a\mathbf{e}_j] - f[\theta]}{a}, \quad (\text{B.3})$$

where a is a small number and \mathbf{e}_j is the unit vector in the j^{th} direction. In principle as a tends to zero, this estimate becomes more accurate. However, in practice the calculation is limited by the floating point precision of the computer, so a must be chosen with care.

B.2.1 Steepest descent

An intuitive way to choose the search direction is to measure the gradient and select the direction which moves us downhill fastest. We could move in this direction until the function no longer decreases, then recompute the steepest direction and move again. In this way, we gradually move toward a local minimum of the function (figure B.3a). The algorithm terminates when the gradient is zero and the second derivative is positive, indicating that we are at the minimum point and any further local changes would not result in further improvement. This approach is termed *steepest descent*. More precisely, we choose

$$\theta^{[t+1]} = \theta^{[t]} - \lambda \left. \frac{\partial f}{\partial \theta} \right|_{\theta^{[t]}}, \quad (\text{B.4})$$

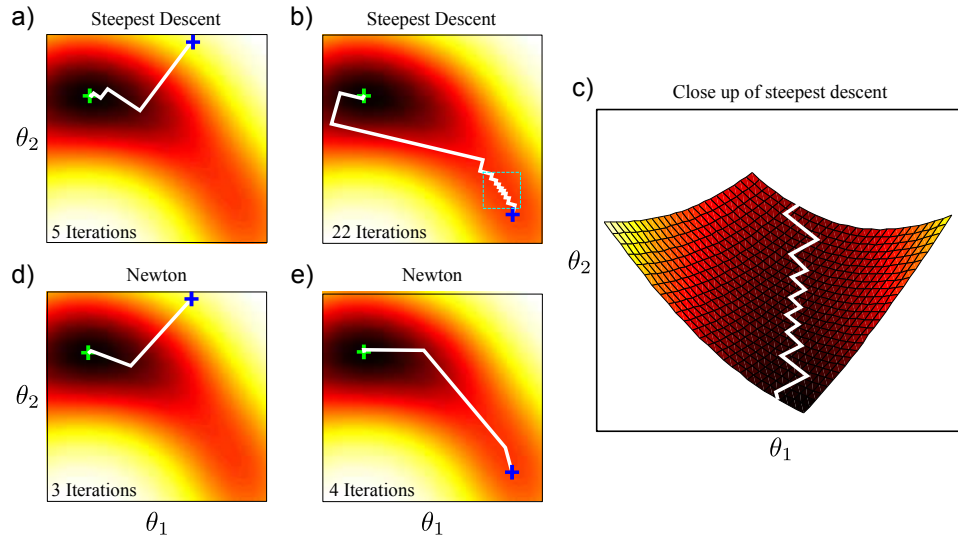


Figure B.3 Optimization on a two dimensional function (color represents height of function). We wish to find the parameters that minimize the function (green cross). Given an initial starting point θ^0 (blue cross), we choose a direction and then perform a local search to find the optimal point in that direction. a) One way to choose the direction is steepest descent: at each iteration, we head in the direction where the function changes the fastest. b) When we initialize from a different position, the steepest descent method takes many iterations to converge due to oscillatory behavior. c) Close-up of oscillatory region (see main text). d) Setting the direction using Newton's method results in faster convergence. e) Newton's method does not undergo oscillatory behavior when we initialize from the second position.

where the derivative $\partial f / \partial \theta$ is the *gradient vector*, which points uphill, and λ is the distance moved downhill in the opposite direction $-\partial f / \partial \theta$. The line search procedure (section B.3) selects the value of λ .

Steepest descent sounds like a good idea but can be very inefficient in certain situations (figure B.3b). For example, in a descending valley, it can oscillate ineffectually from one side to the other rather than proceeding straight down the center: the method approaches the bottom of the valley from one side, but overshoots because the valley itself is descending, so the minimum along the search direction is not exactly in the valley center (figure B.3c). When we re-measure the gradient and perform a second line search, we overshoot in the other direction. This is not an unusual situation: it is guaranteed that the gradient at the new point will be perpendicular to the previous one, so the only way to avoid this oscillation is to hit the valley at exactly right angles.

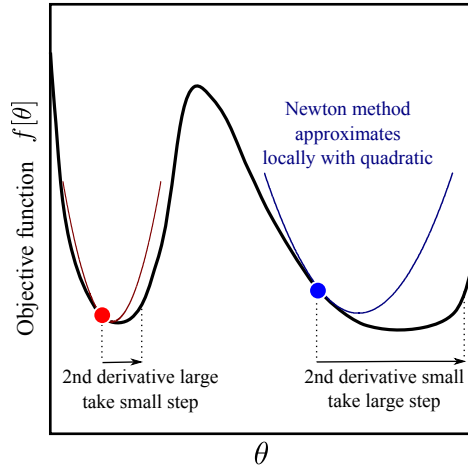


Figure B.4 Use of second derivatives. The gradient at the red and blue points is the same, but the magnitude of the second derivative is larger at the red point than the blue point: the gradient is changing faster at the red point than the blue point. The distance we move should be moderated by the second derivative: if the gradient is changing fast, then the minimum may be nearby and we should move a small distance. If it is changing slowly, then it is safe to move further. Newton's method takes into account the second derivative: it uses a Taylor expansion to create a quadratic approximation to the function and then moves toward the minimum.

B.2.2 Newton's method

Newton's method is an improved approach that also exploits the second derivatives at the current point: it considers both the gradient of the function and how that gradient is changing.

To motivate the use of second derivatives, consider a one-dimensional function (figure B.4). If the magnitude of the second derivative is low, then the gradient is changing slowly. Consequently, it will probably take a while before it completely flattens out and becomes a minimum, and so it is safe to move a long distance. Conversely, if the magnitude of the second derivative is high, then things are changing rapidly, and we should move only a small distance.

Now consider the same argument in two dimensions. Imagine we are at a point where the gradient is identical in both dimensions. For steepest descent, we would move equally in both dimensions. However, if the magnitude of the second derivative in the first direction is much greater than that in the second, we would nonetheless wish to move further in the second direction.

To see how to exploit the second derivatives algebraically, consider a truncated Taylor expansion around the current estimate $\theta^{[t]}$:

$$f[\theta] \approx f[\theta^{[t]}] + (\theta - \theta^{[t]})^T \left. \frac{\partial f}{\partial \theta} \right|_{\theta^{[t]}} + \frac{1}{2} (\theta - \theta^{[t]})^T \left. \frac{\partial^2 f}{\partial \theta^2} \right|_{\theta^{[t]}} (\theta - \theta^{[t]}), \quad (\text{B.5})$$

where θ is a $D \times 1$ variable, the first derivative vector is of size $D \times 1$, and the Hessian matrix of second derivatives is $D \times D$. To find the local extrema, we now take derivatives with respect to θ and set the result to zero

$$\frac{\partial f}{\partial \theta} \approx \left. \frac{\partial f}{\partial \theta} \right|_{\theta^{[t]}} + \left. \frac{\partial^2 f}{\partial \theta^2} \right|_{\theta^{[t]}} (\theta - \theta^{[t]}) = 0. \quad (\text{B.6})$$

By re-arranging this equation, we get an expression for the minimum $\hat{\theta}$,

$$\hat{\theta} = \theta^{[t]} - \left(\frac{\partial^2 f}{\partial \theta^2} \right)^{-1} \frac{\partial f}{\partial \theta}, \quad (\text{B.7})$$

where the derivatives are still taken at $\theta^{[t]}$, but we have stopped writing this for clarity. In practice we would implement Newton's method as a series of iterations

$$\theta^{[t+1]} = \theta^{[t]} - \lambda \left(\frac{\partial^2 f}{\partial \theta^2} \right)^{-1} \frac{\partial f}{\partial \theta}, \quad (\text{B.8})$$

where the λ is the step size. This can be set to one, or we can find the optimal value using line search.

One interpretation of Newton's method is that we have locally approximated the function as a quadratic. On each iteration, we move toward its extremum (or move exactly to it if we fix $\lambda = 1$). Note that we are assuming that we are close enough to the correct solution that the nearby extremum *is* a minimum and not a saddle point or maximum. In particular, if the Hessian is not positive definite then a direction that is not downhill may be chosen. In this sense Newton's method is not as robust as steepest descent.

Subject to this limitation, Newton's method converges in fewer iterations than steepest descent (figure B.3d-e). However, it requires more computation per iteration as we have to invert the $D \times D$ Hessian matrix at each step. Choosing this method usually implies that we can write the Hessian in closed form; approximating the Hessian from finite derivatives requires many function evaluations and so is potentially very costly.

B.2.3 Gauss-Newton method

Cost functions in computer vision often take the special form of a least squares problem

$$f[\theta] = \sum_{i=1}^I (\mathbf{x}_i - \mathbf{g}[\mathbf{w}_i, \theta])^T (\mathbf{x}_i - \mathbf{g}[\mathbf{w}_i, \theta]), \quad (\text{B.9})$$

where $\mathbf{g}[\bullet, \bullet]$ is a function that transfers the variables $\{\mathbf{w}_i\}$ into the space of the variables $\{\mathbf{x}_i\}$, and is parameterized by θ . In other words, we seek the values of θ that most closely map $\{\mathbf{w}_i\}$ to $\{\mathbf{x}_i\}$ in a least squares sense. This cost function is a special case of the more general form $f[\theta] = \mathbf{z}^T \mathbf{z}$, where

$$\mathbf{z} = \begin{bmatrix} \mathbf{x}_1 - \mathbf{g}[\mathbf{w}_1, \theta] \\ \mathbf{x}_2 - \mathbf{g}[\mathbf{w}_2, \theta] \\ \vdots \\ \mathbf{x}_I - \mathbf{g}[\mathbf{w}_I, \theta] \end{bmatrix}. \quad (\text{B.10})$$

The *Gauss-Newton method* is an optimization technique that is used to solve least squares problems of the form

$$\hat{\theta} = \operatorname{argmin} [f[\theta]] \quad \text{where } f[\theta] = \mathbf{z}[\theta]^T \mathbf{z}[\theta]. \quad (\text{B.11})$$

To minimize this objective function, we approximate the term $\mathbf{z}[\boldsymbol{\theta}]$ with a Taylor series expansion around the current estimate $\boldsymbol{\theta}^{[t]}$ of the parameters:

$$\mathbf{z}[\boldsymbol{\theta}] \approx \mathbf{z}[\boldsymbol{\theta}^{[t]}] + \mathbf{J}(\boldsymbol{\theta} - \boldsymbol{\theta}^{[t]}), \quad (\text{B.12})$$

where \mathbf{J} is the Jacobian matrix. The entry j_{mn} at the m^{th} row and the n^{th} column of \mathbf{J} contains the derivative of the m^{th} element of \mathbf{z} with respect to the n^{th} parameter so that

$$j_{mn} = \frac{\partial z_m}{\partial \theta_n}. \quad (\text{B.13})$$

Now we substitute the approximation for $\mathbf{z}[\boldsymbol{\theta}]$ into the original cost function $f[\boldsymbol{\theta}] = \mathbf{z}^T \mathbf{z}$ to yield

$$\begin{aligned} f[\boldsymbol{\theta}] &\approx (\mathbf{z}[\boldsymbol{\theta}^{[t]}] + \mathbf{J}(\boldsymbol{\theta} - \boldsymbol{\theta}^{[t]}))^T (\mathbf{z}[\boldsymbol{\theta}^{[t]}] + \mathbf{J}(\boldsymbol{\theta} - \boldsymbol{\theta}^{[t]})) \\ &= \mathbf{z}[\boldsymbol{\theta}^{[t]}]^T \mathbf{z}[\boldsymbol{\theta}^{[t]}] + 2(\boldsymbol{\theta} - \boldsymbol{\theta}^{[t]})^T \mathbf{J}^T \mathbf{z}[\boldsymbol{\theta}^{[t]}] + (\boldsymbol{\theta} - \boldsymbol{\theta}^{[t]})^T \mathbf{J}^T \mathbf{J} (\boldsymbol{\theta} - \boldsymbol{\theta}^{[t]}). \end{aligned} \quad (\text{B.14})$$

Finally, we take derivatives of this expression with respect to the parameters $\boldsymbol{\theta}$ and equate to zero to get the relation

$$\frac{\partial f}{\partial \boldsymbol{\theta}} \approx 2\mathbf{J}^T \mathbf{z}[\boldsymbol{\theta}^{[t]}] + 2\mathbf{J}^T \mathbf{J} (\boldsymbol{\theta} - \boldsymbol{\theta}^{[t]}) = 0. \quad (\text{B.15})$$

Re-arranging, we get the update rule:

$$\boldsymbol{\theta} = \boldsymbol{\theta}^{[t]} - (\mathbf{J}^T \mathbf{J})^{-1} \mathbf{J}^T \mathbf{z}[\boldsymbol{\theta}^{[t]}]. \quad (\text{B.16})$$

We can rewrite this by noting that

$$\left. \frac{\partial f}{\partial \boldsymbol{\theta}} \right|_{\boldsymbol{\theta}^{[t]}} = \left. \frac{\partial \mathbf{z}^T \mathbf{z}}{\partial \boldsymbol{\theta}} \right|_{\boldsymbol{\theta}^{[t]}} = 2\mathbf{J}^T \mathbf{z}[\boldsymbol{\theta}^{[t]}], \quad (\text{B.17})$$

to give the final Gauss-Newton update

$$\boldsymbol{\theta}^{[t+1]} = \boldsymbol{\theta}^{[t]} - \lambda (\mathbf{J}^T \mathbf{J})^{-1} \left. \frac{\partial f}{\partial \boldsymbol{\theta}} \right|_{\boldsymbol{\theta}^{[t]}}, \quad (\text{B.18})$$

where the derivative is taken at $\boldsymbol{\theta}^{[t]}$ and λ is the step size.

Comparing with the Newton update (equation B.8), we see that we can consider this update as approximating the Hessian matrix as $\mathbf{H} \approx \mathbf{J}^T \mathbf{J}$. It provides better results than gradient descent without ever computing second derivatives. Moreover, the term $\mathbf{J}^T \mathbf{J}$ is normally positive definite resulting in increased stability.

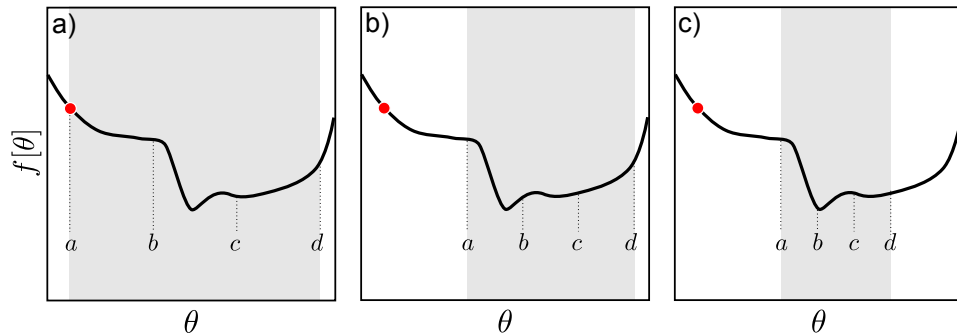


Figure B.5 Line search over region $[a, d]$ using bracketing approach. Gray region indicates current search region. a) We define two points b, c that are interior to the search region and evaluate the function at these points. Here $f[b] > f[c]$ so we eliminate the range $[a, b]$. b) We evaluate two points $[b, c]$ interior to the new range and compare their values. This time we find that $f[b] < f[c]$ so we eliminate the range $[c, d]$. c) We repeat this process until the minimum is closely bracketed.

B.2.4 Other methods

There are numerous other methods for choosing the optimization direction. Many of these involve approximating the Hessian in some way with the goal of either ensuring that a downhill direction is always chosen or reducing the computational burden. For example, if computation of the Hessian is prohibitive, a practical approach is to approximate it with its own diagonal. This usually provides a better direction than steepest descent.

Quasi-Newton methods such as the *Broyden Fletcher Goldfarb Shanno (BFGS) method* approximate the Hessian with information gathered by analyzing successive gradient vectors. The *Levenberg-Marquardt* algorithm interpolates between the Gauss-Newton algorithm and steepest descent with the aim of producing a method that requires few iterations and is also robust. *Damped Newton* and *trust-region methods* also attempt to improve the robustness of Newton's method. The *nonlinear conjugate gradient algorithm* is another valuable method when only first derivatives are available.

B.3 Line search

Having chosen a sensible direction using steepest descent, Newton's method or some other approach, we must now decide how far to move: we need an efficient method to find the minimum of the function in the chosen direction. Line search methods start by determining the range over which to search for the minimum.

This is usually guided by the magnitude of the second derivative along the line, which provides information about the likely search range (see figure B.4).

There are many heuristics to find the minimum, but we will discuss only the direct search method (figure B.5). Consider searching over the region $[a, d]$. We compute the function at two internal points b and c where $a < b < c < d$. If $f[b] < f[c]$, we eliminate the range $[c, d]$ and search over the new region $[a, c]$ at the next iteration. Conversely, if $f[b] > f[c]$, we eliminate the range $[a, b]$ and search over a new region $[b, d]$.

This method is applied iteratively until the minimum is closely bracketed. It is typically not worth exactly locating the minimum; the line search direction is rarely optimal and so the minimum of the line search is usually far from the overall minimum of the function. Once the remaining interval is sufficiently small, an estimate of the minimum position can be computed by making a parabolic fit to the three points that remain after eliminating one region or the other and selecting the position of the minimum of this parabola.

B.4 Reparameterization

Often in vision problems, we must find the best parameters θ subject to one or more constraints. Typical examples include optimizing variances σ^2 which must be positive, covariance matrices, which must be positive definite, and matrices that represent geometric rotations, which must be orthogonal. The general topic of constrained optimization is beyond the scope of this volume, but we briefly describe a trick that can be used to convert constrained optimization problems into unconstrained ones, which can be solved using the techniques already described.

The idea of reparameterization is to represent the parameters θ in terms of a new set of parameters ϕ , which do not have any constraints on them, so that

$$\theta = \mathbf{g}[\phi], \quad (\text{B.19})$$

where $\mathbf{g}[\bullet]$ is a carefully chosen function.

Then we optimize with respect to the new unconstrained parameters ϕ . The objective function becomes $f[\mathbf{g}[\phi]]$ and the derivatives are computed using the chain rule so that the first derivative would be

$$\frac{\partial f}{\partial \phi} = \sum_{k=1}^K \frac{\partial f}{\partial \theta_k} \frac{\partial \theta_k}{\partial \phi}. \quad (\text{B.20})$$

where θ_k is the k^{th} element of θ . This strategy is easier to understand with some concrete examples.

Parameters that must be positive

When we optimize a variance parameter $\theta = \sigma^2$ we must ensure that the final answer is positive. To this end, we use the relation:

$$\theta = \exp[\phi], \quad (\text{B.21})$$

and now optimize with respect to the new scalar parameter ϕ . Alternatively, we can use the square relation:

$$\theta = \phi^2, \quad (\text{B.22})$$

and again optimize with respect to the parameter ϕ .

Parameters that must lie between 0 and 1

To ensure that a scalar parameter θ lies between zero and one, we use the logistic sigmoid function:

$$\theta = \frac{1}{1 + \exp[-\phi]}, \quad (\text{B.23})$$

and optimize with respect to the new scalar parameter ϕ .

Parameters that must be positive and sum to one

To ensure that the elements of a $K \times 1$ multivariable parameter θ sum to one and are all positive we use the softmax function:

$$\theta_k = \frac{\exp[\phi_k]}{\sum_{j=1}^K \exp[\phi_j]}, \quad (\text{B.24})$$

and optimize with respect to the new $K \times 1$ variable ϕ .

3D rotation matrices

A 3×3 rotation matrix contains three independent quantities spread throughout its nine entries. A number of nonlinear constraints exist between the entries: the norm of each column and row must be one, each column is perpendicular to the other columns, each row is perpendicular to the other rows, and the determinant is one.

One way to enforce these constraints is to re-parameterize the rotation matrix as a *quaternion* and optimize with respect to this new representation. A quaternion \mathbf{q} is a 4D quantity $\mathbf{q} = [q_0, q_1, q_2, q_3]$. Mathematically speaking, they are a four dimensional extension of complex numbers, but the relevance for vision is that they can be used to represent 3D rotations. We use the relation:

$$\Theta = \frac{1}{q_0^2 + q_1^2 + q_2^2 + q_3^2} \begin{bmatrix} q_0^2 + q_1^2 - q_2^2 - q_3^2 & 2q_1q_2 - 2q_0q_3 & 2q_1q_3 + 2q_0q_2 \\ 2q_1q_2 + 2q_0q_3 & q_0^2 - q_1^2 + q_2^2 - q_3^2 & 2q_2q_3 - 2q_0q_1 \\ 2q_1q_3 - 2q_0q_2 & 2q_2q_3 + 2q_0q_1 & q_0^2 - q_1^2 - q_2^2 + q_3^2 \end{bmatrix}. \quad (\text{B.25})$$

Although the quaternion contains four numbers, only the ratios of those numbers are important (giving 3 degrees of freedom): each element of equation B.25

consists of squared terms, which are normalized by the squared amplitude constant, and so any constant that multiplies the elements of \mathbf{q} is canceled out when we convert back to a rotation matrix.

Now we optimize with respect to the quaternion \mathbf{q} . The derivatives with respect to the k^{th} element of \mathbf{q} can be computed as

$$\frac{\partial f}{\partial q_k} = \sum_{i=1}^3 \sum_{j=1}^3 \frac{\partial f}{\partial \Theta_{ij}} \frac{\partial \Theta_{ij}}{\partial q_k}. \quad (\text{B.26})$$

The quaternion optimization is stable as long as we do not approach the singularity at $\mathbf{q} = \mathbf{0}$. One way to achieve this is to periodically re-normalize the quaternion to length 1 during the optimization procedure.

Positive definite matrices

When we optimize over a $K \times K$ covariance matrix $\Theta = \Sigma$, we must ensure that the result is positive definite. A simple way to do this is to use the relation:

$$\Theta = \Phi \Phi^T, \quad (\text{B.27})$$

where Φ is an arbitrary $K \times K$ matrix.

Appendix C

Linear algebra

C.1 Vectors

A vector is a geometric entity in D dimensional space that has both a direction and a magnitude. It is represented by a $D \times 1$ array of numbers. In this book, we write vectors as bold, small, Roman or Greek letters (e.g., \mathbf{a}, ϕ). The transpose \mathbf{a}^T of vector \mathbf{a} is a $1 \times D$ array of numbers where the order of the numbers is retained.

C.1.1 Dot product

The *dot product* or *scalar product* between two vectors \mathbf{a} and \mathbf{b} is defined as

$$c = \mathbf{a}^T \mathbf{b} = \sum_{d=1}^D a_d b_d, \quad (\text{C.1})$$

where \mathbf{a}^T is the transpose of \mathbf{a} (i.e., \mathbf{a} converted to a row vector) and the returned value c is a scalar. Two vectors are said to be *orthogonal* if the dot product between them is zero.

C.1.2 Norm of a vector

The *magnitude* or *norm* of a vector is the square root of the sum of the square of the D elements so that,

$$\text{norm}[\mathbf{a}] = |\mathbf{a}| = \left(\sum_{d=1}^D a_d^2 \right)^{1/2} = (\mathbf{a}^T \mathbf{a})^{1/2}. \quad (\text{C.2})$$

C.1.3 Cross product

The *cross product* or *vector product* is specialized to three dimensions. The operation $\mathbf{c} = \mathbf{a} \times \mathbf{b}$ is equivalent to the matrix multiplication (section C.2.1):

$$\begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} 0 & -a_3 & a_2 \\ a_3 & 0 & -a_1 \\ -a_2 & a_1 & 0 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}, \quad (\text{C.3})$$

or for short

$$\mathbf{c} = \mathbf{A}_\times \mathbf{b}, \quad (\text{C.4})$$

where \mathbf{A}_\times is the 3×3 matrix from equation C.3 that implements the cross product.

It is easily shown that the result \mathbf{c} of the cross product is orthogonal to both \mathbf{a} and \mathbf{b} . In other words,

$$\mathbf{a}^T(\mathbf{a} \times \mathbf{b}) = \mathbf{b}^T(\mathbf{a} \times \mathbf{b}) = 0. \quad (\text{C.5})$$

C.2 Matrices

Matrices are used extensively throughout the book and are written as bold, capital, Roman or Greek letters (e.g., \mathbf{A}, Φ). We categorize matrices as *landscape* (more columns than rows), *square* (the same number of columns and rows) or *portrait* (more rows than columns). They are always indexed by row first and then column, so a_{ij} denotes the element of matrix \mathbf{A} at the i^{th} row and the j^{th} column.

A *diagonal* matrix is a square matrix with zeros everywhere except on the diagonal (i.e., elements a_{ii}) where the elements may take any value. An important special case of a diagonal matrix is the *identity* matrix \mathbf{I} . This has zeros everywhere except for the diagonal, where all the elements are ones.

C.2.1 Matrix multiplication

To take the matrix product $\mathbf{C} = \mathbf{AB}$, we compute the elements of \mathbf{C} as

$$c_{ij} = \sum_{k=1}^K a_{ik} b_{kj}. \quad (\text{C.6})$$

This can only be done when the number of columns in \mathbf{A} equals the number of rows in \mathbf{B} . Matrix multiplication is associative so that $\mathbf{A}(\mathbf{BC}) = (\mathbf{AB})\mathbf{C} = \mathbf{ABC}$. However it is not commutative so that in general $\mathbf{AB} \neq \mathbf{BA}$.

C.2.2 Transpose

The transpose of a matrix \mathbf{A} is written as \mathbf{A}^T and is formed by reflecting it around the principal diagonal, so that the k^{th} column becomes the k^{th} row and vice-versa. If we take the transpose of a matrix product \mathbf{AB} , then we take the transpose of the original matrices but reverse the order so that

$$(\mathbf{AB})^T = \mathbf{B}^T \mathbf{A}^T. \quad (\text{C.7})$$

C.2.3 Inverse

A square matrix \mathbf{A} may or may not have an inverse \mathbf{A}^{-1} such that $\mathbf{A}^{-1}\mathbf{A} = \mathbf{AA}^{-1} = \mathbf{I}$. If a matrix does not have an inverse, it is called *singular*.

Diagonal matrices are particularly easy to invert: the inverse is also a diagonal matrix, with each diagonal value d_{ii} replaced by $1/d_{ii}$. Hence, any diagonal matrix that has non-zero values on the diagonal is invertible. It follows that the inverse of the identity matrix is the identity matrix itself.

If we take the inverse of a matrix product \mathbf{AB} , then we can equivalently take the inverse of each matrix individually, and reverse the order of multiplication

$$(\mathbf{AB})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1}. \quad (\text{C.8})$$

C.2.4 Determinant and trace

Every square matrix \mathbf{A} has a scalar associated with it called the determinant, denoted by $|\mathbf{A}|$ or $\det[\mathbf{A}]$. It is (loosely) related to the scaling applied by the matrix. As a rule of thumb, matrices where the magnitude of the determinant is small tend to make vectors smaller upon multiplication and matrices where the magnitude of the determinant is large tend to make them larger. If a matrix is singular, the determinant will be zero and there will be at least one direction in space that is mapped to the origin when the matrix is applied. For a diagonal matrix, the determinant is the product of the diagonal values. It follows that the determinant of the identity matrix is 1. Determinants of matrix expressions can be computed using the following rules:

$$|\mathbf{A}^T| = |\mathbf{A}| \quad (\text{C.9})$$

$$|\mathbf{AB}| = |\mathbf{A}||\mathbf{B}| \quad (\text{C.10})$$

$$|\mathbf{A}^{-1}| = 1/|\mathbf{A}|. \quad (\text{C.11})$$

The trace of a matrix is a second number associated with a square matrix \mathbf{A} . It is the sum of the diagonal values (the matrix itself need not be diagonal). The traces of compound terms are bound by the following rules:

$$\text{tr}[\mathbf{A}^T] = \text{tr}[\mathbf{A}] \quad (\text{C.12})$$

$$\text{tr}[\mathbf{AB}] = \text{tr}[\mathbf{BA}] \quad (\text{C.13})$$

$$\text{tr}[\mathbf{A} + \mathbf{B}] = \text{tr}[\mathbf{A}] + \text{tr}[\mathbf{B}] \quad (\text{C.14})$$

$$\text{tr}[\mathbf{ABC}] = \text{tr}[\mathbf{BCA}] = \text{tr}[\mathbf{CAB}], \quad (\text{C.15})$$

where in the last relation, the trace is invariant for cyclic permutations only, so that in general $\text{tr}[\mathbf{ABC}] \neq \text{tr}[\mathbf{BAC}]$.

C.2.5 Orthogonal and rotation matrices

An important class of square matrix is the orthogonal matrix. Orthogonal matrices have the following special properties:

1. Each column has norm one, and each row has norm one.
2. Each column is orthogonal to every other column, and each row is orthogonal to every other row.

The inverse of an orthogonal matrix $\mathbf{\Omega}$ is its own transpose, so $\mathbf{\Omega}^T \mathbf{\Omega} = \mathbf{\Omega}^{-1} \mathbf{\Omega} = \mathbf{I}$; orthogonal matrices are easy to invert! When this class of matrix pre-multiplies a vector, the effect is to rotate it around the origin and possibly reflect it.

Rotation matrices are a sub-class of orthogonal matrices that have the additional property that the determinant is one. As the name suggests, when this class of matrix pre-multiplies a vector, the effect is to rotate it around the origin with no reflection.

C.2.6 Positive definite matrices

A $D \times D$ real symmetric matrix \mathbf{A} is *positive definite* if $\mathbf{x}^T \mathbf{A} \mathbf{x} > 0$ for all non-zero vectors \mathbf{x} . Every positive definite matrix is invertible and its inverse is also positive definite. The determinant and trace of a symmetric positive definite matrix are always positive. The covariance matrix $\mathbf{\Sigma}$ of a normal distribution is always positive definite.

C.2.7 Null space of a matrix

The right null space of a matrix \mathbf{A} consists of the set of vectors \mathbf{x} for which

$$\mathbf{A} \mathbf{x} = \mathbf{0}. \quad (\text{C.16})$$

Similarly, the left null space of a matrix \mathbf{A} consists of the set of vectors \mathbf{x} for which

$$\mathbf{x}^T \mathbf{A} = \mathbf{0}^T. \quad (\text{C.17})$$

A square matrix only has a non-trivial null space (i.e., not just $\mathbf{x} = \mathbf{0}$) if the matrix is singular (non-invertible) and hence the determinant is zero.

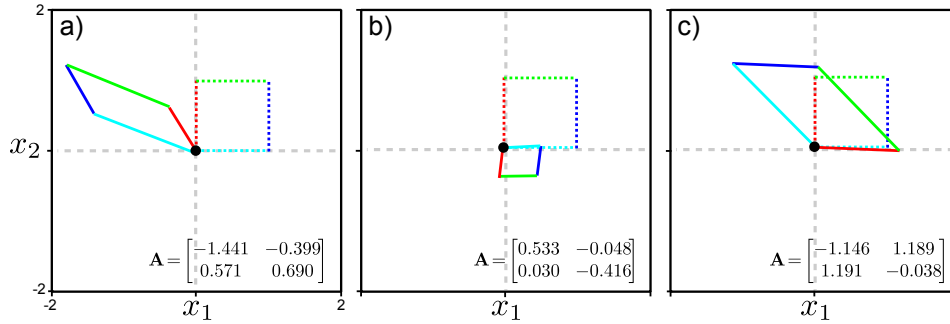


Figure C.1 Effect of applying three linear transformations to a unit square. Dashed square is before transformation. Solid square is after. The origin is always mapped to the origin. Co-linear points remain co-linear. Parallel lines remain parallel. The linear transformation encompasses shears, reflections, rotations and scalings.

C.3 Tensors

We will occasionally have need for $D > 2$ dimensional quantities that we shall refer to as D -dimensional tensors. For our purposes a matrix can be thought of as the special case of a 2 dimensional tensor, and a vector as the special case of a 1D tensor.

The idea of taking matrix products generalizes to higher dimensions and is denoted using the special notion \times_n where n is the dimension over which we take the product. For example, the l^{th} element f_l of the tensor product $\mathbf{f} = \mathbf{A} \times_2 \mathbf{b} \times_3 \mathbf{c}$ is given by

$$f_l = \sum_m \sum_n A_{lmn} b_m c_n, \quad (\text{C.18})$$

where l , m and n index the 3D tensor \mathbf{A} , and \mathbf{b} and \mathbf{c} are vectors.

C.4 Linear transformations

When we pre-multiply a vector by a matrix this is called a linear transformation. Figure C.1 shows the results of applying several different 2D linear transformations (randomly chosen 2×2 matrices) to the 2D vectors that represent the points of the unit square. We can deduce several things from this figure. First, the point (0,0) at the origin is always mapped back onto itself. Second, collinear points remain collinear. Third, parallel lines are always mapped to parallel lines. Viewed as a geometric transformation, pre-multiplication by a matrix can account for shearing, scaling, reflection and rotation around the origin.

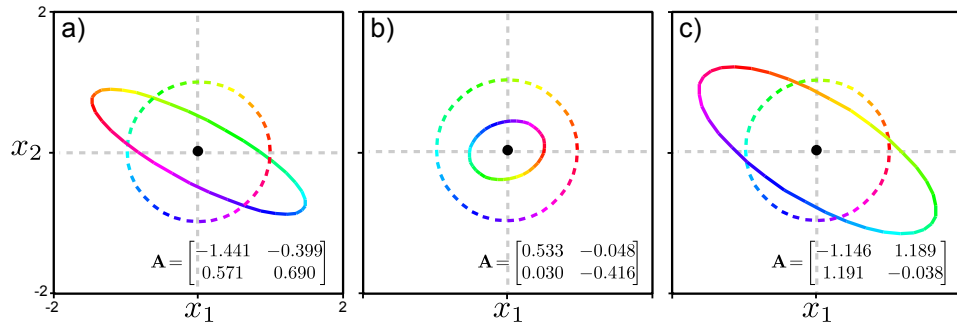


Figure C.2 Effect of applying three linear transformations to a circle. Dashed circle is before transformation. Solid ellipse is after. After the transformation, the circle is mapped to an ellipse. This demonstrates that there is one special direction that is expanded the most (becomes the major axis of the ellipse), and one special direction that is expanded the least (becomes the minor axis of the ellipse).

A different perspective on linear transforms comes from applying different transformations to points on the unit circle (figure C.2). In each case, the circle is transformed to an ellipse. The ellipse can be characterized by its major axis (most elongated axis) and its minor axis (most compact axis), which are perpendicular to one another. This tells us something interesting: in general, there is a special direction in space (position on the original circle) that gets stretched the most (or compressed the least) by the transformation. Likewise there is a second direction that gets stretched the least or compressed the most.

C.5 Singular value decomposition

The singular value decomposition (SVD) is a factorization of a $M \times N$ matrix \mathbf{A} , such that

$$\mathbf{A} = \mathbf{U}\mathbf{L}\mathbf{V}^T, \quad (\text{C.19})$$

where \mathbf{U} is a $M \times M$ orthogonal matrix, \mathbf{L} is a $M \times N$ diagonal matrix, and \mathbf{V} is a $N \times N$ orthogonal matrix. It is always possible to compute this factorization, although a description of how to do so is beyond the scope of this book.

The best way to get the flavor of the SVD is to consider some examples. First let us consider a square matrix:

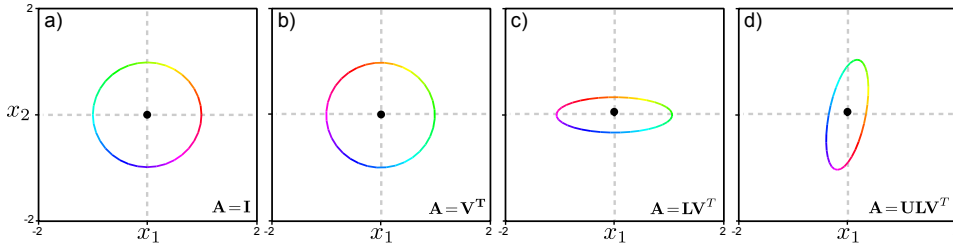


Figure C.3 Cumulative effect of SVD components for matrix \mathbf{A}_3 . a) Original object. b) Applying matrix \mathbf{V}^T rotates and reflects the object around the origin. c) Subsequently applying \mathbf{L} causes stretching/compression along the coordinate axes. d) Finally, applying matrix \mathbf{U} rotates and reflects this distorted structure.

$$\begin{aligned}\mathbf{A}_1 &= \begin{bmatrix} 0.183 & 0.307 & 0.261 \\ -1.029 & 0.135 & -0.941 \\ 0.949 & 0.515 & -0.162 \end{bmatrix} = \mathbf{U}\mathbf{L}\mathbf{V}^T \\ &= \begin{bmatrix} -0.204 & -0.061 & -0.977 \\ 0.832 & -0.535 & -0.140 \\ -0.514 & -0.842 & 0.160 \end{bmatrix} \begin{bmatrix} 1.590 & 0 & 0 \\ 0 & 0.856 & 0 \\ 0 & 0 & 0.303 \end{bmatrix} \begin{bmatrix} -0.870 & -0.302 & 0.389 \\ -0.135 & -0.613 & -0.778 \\ -0.474 & 0.729 & -0.492 \end{bmatrix}.\end{aligned}\quad (\text{C.20})$$

Notice that by convention, the non-negative values on the principal diagonal of \mathbf{L} decrease monotonically as we move from top-left to bottom-right. These are known as the *singular values*.

Now consider the singular value decomposition of a portrait matrix:

$$\begin{aligned}\mathbf{A}_2 &= \begin{bmatrix} 0.537 & 0.862 \\ 1.839 & 0.318 \\ -2.258 & -1.307 \end{bmatrix} = \mathbf{U}\mathbf{L}\mathbf{V}^T \\ &= \begin{bmatrix} -0.263 & 0.698 & 0.665 \\ -0.545 & -0.676 & 0.493 \\ 0.795 & -0.233 & 0.559 \end{bmatrix} \begin{bmatrix} 3.273 & 0 \\ 0 & 0.76 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} -0.898 & -0.440 \\ -0.440 & 0.898 \end{bmatrix}.\end{aligned}\quad (\text{C.21})$$

For this rectangular matrix, the orthogonal matrices \mathbf{U} and \mathbf{V} are different sizes and the diagonal matrix \mathbf{L} is the same size as the original matrix. The singular values are still found on the diagonal, but the number is determined by the smallest dimension. In other words, if the original matrix was $M \times N$ then there will be $\min[M, N]$ singular values.

To further understand the SVD, let us consider a third example:

$$\mathbf{A}_3 = \begin{bmatrix} -0.147 & 0.357 \\ -0.668 & 0.811 \end{bmatrix} = \begin{bmatrix} 0.189 & 0.981 \\ 0.981 & -0.189 \end{bmatrix} \begin{bmatrix} 1.068 & 0 \\ 0 & 0.335 \end{bmatrix} \begin{bmatrix} -0.587 & 0.8091 \\ 0.809 & 0.587 \end{bmatrix}. \quad (\text{C.22})$$

Figure C.3 illustrates the cumulative effect of the transformations in the decomposition $\mathbf{A}_3 = \mathbf{U}\mathbf{L}\mathbf{V}^T$. The matrix \mathbf{V}^T rotates and reflects the original points. The matrix \mathbf{L} scales the result differently along each dimension. In this case it is stretched along the first dimension and shrunk along the second. Finally, the matrix \mathbf{U} rotates the result.

Figure C.4 provides a second perspective on this process. Each pair of panels depicts what happens when we modify a different part of the SVD but keep the remaining parts the same. When we change \mathbf{V} , the shape of the final ellipse is the same, but the mapping from original directions to points on the ellipse changes (observe the color change along the major axis). When we modify the first element of \mathbf{L} , the length of the major axis changes. When we change the other non-zero element of \mathbf{L} , the length of the minor axis changes. When we change the matrix \mathbf{U} , the orientation of the ellipse changes.

C.5.1 Analyzing the singular values

We can learn a lot about a matrix by looking at the singular values. We saw in the previous section, that as we decrease the smallest singular value the minor axis of the ellipse becomes progressively smaller. When it actually becomes zero, both sides of the unit circle collapse into one another (as do points from circles of all radii). Now there is a many-to-one mapping from the original points to the transformed ones, and the matrix is no longer invertible. In general, a matrix is only invertible if all of the singular values are non-zero.

The number of non-zero singular values is called the rank of the matrix. The ratio of the smallest to the largest singular values is known as the condition number: it is roughly a measure of how ‘invertible’ the matrix is. As it becomes close to zero, our ability to invert the matrix decreases.

The singular values scale the different axes of the ellipse by different amounts (figure C.3c). Hence, the area of a unit circle is changed by a factor that is equal to the product of the singular values. In fact this scaling factor is the determinant (section C.2.4). When the matrix is singular, at least one of the singular values is zero and hence the determinant is also zero. The right null space consists of all of the vectors that can be reached by taking a weighted sum of those columns of \mathbf{V} whose corresponding singular values are zero. Similarly, the left null space consists of all of the vectors that can be reached by taking a weighted sum of those columns of \mathbf{U} whose corresponding singular values are zero.

Orthogonal matrices only rotate and reflect points, and rotation matrices just rotate them. In either case, there is no change in area to the unit circle: all the singular values are one for these matrices and the determinant is also one.

C.5.2 Inverse of a matrix

We can also see what happens when we invert a square matrix in terms of the singular value decomposition. Using the rule $(\mathbf{AB})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1}$, we have

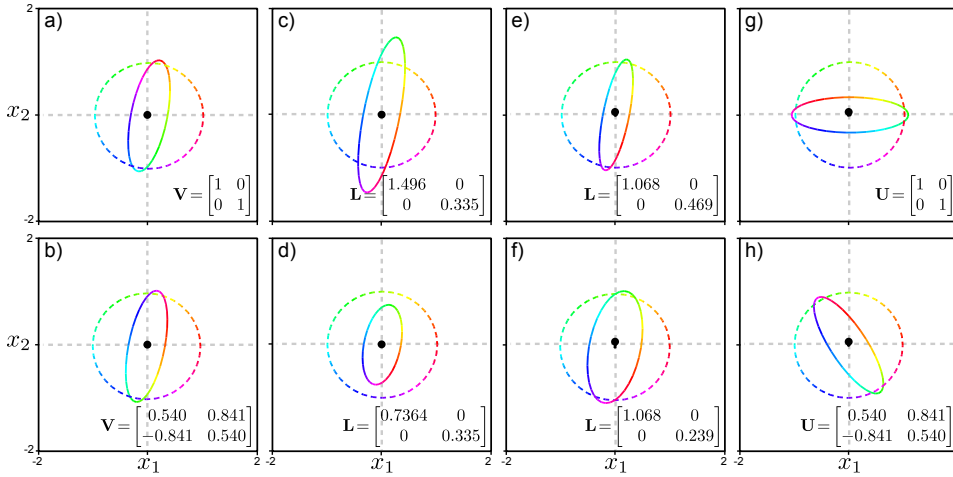


Figure C.4 Manipulating different parts of the SVD of \mathbf{A}_3 . a-b) Changing matrix \mathbf{V} does not affect the final ellipse, but changes which directions (colors) are mapped to the minor and major axes. c-d) Changing the first diagonal element of \mathbf{L} changes the length of the major axis of the ellipse. e-f) Changing the second diagonal element of \mathbf{L} changes the length of the minor axis. g-h) Changing \mathbf{U} affects the final orientation of the ellipse.

$$\mathbf{A}^{-1} = (\mathbf{U}\mathbf{L}\mathbf{V}^T)^{-1} = (\mathbf{V}^T)^{-1}\mathbf{L}^{-1}\mathbf{U}^{-1} = \mathbf{V}\mathbf{L}^{-1}\mathbf{U}^T, \quad (\text{C.23})$$

where we have used the fact that \mathbf{U} and \mathbf{V} are orthogonal matrices so $\mathbf{U}^{-1} = \mathbf{U}^T$ and $\mathbf{V}^{-1} = \mathbf{V}^T$. The matrix \mathbf{L} is diagonal so \mathbf{L}^{-1} will also be diagonal with new non-zero entries that are the reciprocal of the original values. This also shows that the matrix is not invertible when any of the singular values are zero: we cannot take the reciprocal of 0.

Expressed in this way, the inverse has the opposite geometric effect to that of the original matrix: if we consider the effect on the transformed ellipse in figure C.3d, it first rotates by \mathbf{U}^T so its major and minor axis are aligned with the coordinate axes (figure C.3c). Then it scales these axes (using the elements of \mathbf{L}^{-1}), so that the ellipse becomes a circle (figure C.3b). Finally, it rotates the result by \mathbf{V} to get back to the original position (figure C.3a).

C.6 Matrix calculus

We are often called upon to take derivatives of compound matrix expressions. The derivative of a function $f[\mathbf{a}]$ that takes a vector as its argument and returns a scalar is a vector \mathbf{b} with elements

$$b_i = \frac{\partial f}{\partial a_i} \quad (\text{C.24})$$

The derivative of a function $f[\mathbf{A}]$ that returns a scalar, with respect to an $M \times N$ matrix \mathbf{A} will be a $M \times N$ matrix \mathbf{B} with elements

$$b_{ij} = \frac{\partial f}{\partial a_{ij}}. \quad (\text{C.25})$$

The derivative of a function $\mathbf{f}[\mathbf{a}]$ that returns a vector with respect to vector \mathbf{a} is a matrix \mathbf{B} with elements

$$b_{ij} = \frac{\partial f_i}{\partial a_j}. \quad (\text{C.26})$$

where f_i is the i^{th} element of the vector returned by the function $\mathbf{f}[\mathbf{a}]$.

We now provide several commonly used results for reference.

1. Derivative of linear function:

$$\frac{\partial \mathbf{x}^T \mathbf{a}}{\partial \mathbf{x}} = \mathbf{a} \quad (\text{C.27})$$

$$\frac{\partial \mathbf{a}^T \mathbf{x}}{\partial \mathbf{x}} = \mathbf{a} \quad (\text{C.28})$$

$$\frac{\partial \mathbf{a}^T \mathbf{X} \mathbf{b}}{\partial \mathbf{X}} = \mathbf{a} \mathbf{b}^T \quad (\text{C.29})$$

$$\frac{\partial \mathbf{a}^T \mathbf{X}^T \mathbf{b}}{\partial \mathbf{X}} = \mathbf{b} \mathbf{a}^T. \quad (\text{C.30})$$

2. Derivative of quadratic function:

$$\frac{\partial \mathbf{b}^T \mathbf{X}^T \mathbf{X} \mathbf{c}}{\partial \mathbf{X}} = \mathbf{X}(\mathbf{b} \mathbf{c}^T + \mathbf{c} \mathbf{b}^T) \quad (\text{C.31})$$

$$\frac{\partial (\mathbf{B} \mathbf{x} + \mathbf{b})^T \mathbf{C} (\mathbf{D} \mathbf{x} + \mathbf{d})}{\partial \mathbf{x}} = \mathbf{B}^T \mathbf{C} (\mathbf{D} \mathbf{x} + \mathbf{d}) + \mathbf{D}^T \mathbf{C}^T (\mathbf{B} \mathbf{x} + \mathbf{b}) \quad (\text{C.32})$$

$$\frac{\partial \mathbf{x}^T \mathbf{B} \mathbf{x}}{\partial \mathbf{x}} = (\mathbf{B} + \mathbf{B}^T) \mathbf{x} \quad (\text{C.33})$$

$$\frac{\partial \mathbf{b}^T \mathbf{X}^T \mathbf{D} \mathbf{X} \mathbf{c}}{\partial \mathbf{X}} = \mathbf{D}^T \mathbf{X} \mathbf{b} \mathbf{c}^T + \mathbf{D} \mathbf{X} \mathbf{c} \mathbf{b}^T \quad (\text{C.34})$$

$$\frac{\partial (\mathbf{X} \mathbf{b} + \mathbf{c})^T \mathbf{D} (\mathbf{X} \mathbf{b} + \mathbf{c})}{\partial \mathbf{X}} = (\mathbf{D} + \mathbf{D}^T) (\mathbf{X} \mathbf{b} + \mathbf{c}) \mathbf{b}^T. \quad (\text{C.35})$$

3. Derivative of determinant:

$$\frac{\partial \det[\mathbf{Y}]}{\partial x} = \det[\mathbf{Y}] \text{tr} \left[\mathbf{Y}^{-1} \frac{\partial \mathbf{Y}}{\partial x} \right], \quad (\text{C.36})$$

which leads to the relation

$$\frac{\partial \det[\mathbf{Y}]}{\partial \mathbf{Y}} = \det[\mathbf{Y}] \mathbf{Y}^{-T}. \quad (\text{C.37})$$

4. Derivative of log determinant:

$$\frac{\partial \log[\det[\mathbf{Y}]]}{\partial \mathbf{Y}} = \mathbf{Y}^{-T}. \quad (\text{C.38})$$

5. Derivative of inverse:

$$\frac{\partial \mathbf{Y}^{-1}}{\partial x} = -\mathbf{Y}^{-1} \frac{\partial \mathbf{Y}}{\partial x} \mathbf{Y}^{-1}. \quad (\text{C.39})$$

6. Derivative of trace:

$$\frac{\partial \text{tr}[\mathbf{F}[\mathbf{X}]]}{\partial \mathbf{X}} = \left(\frac{\partial \mathbf{F}[\mathbf{X}]}{\partial \mathbf{X}} \right)^T. \quad (\text{C.40})$$

More information about matrix calculus can be found in Petersen *et al.* (2006).

C.7 Common problems

In this section, we discuss several standard linear algebra problems that are found repeatedly in computer vision.

C.7.1 Least squares problems

Many inference and learning tasks in computer vision result in least squares problems. The most frequent context is when we use maximum likelihood methods with the normal distribution. The least squares problem may be formulated in a number of ways. We may be asked to find the vector \mathbf{x} that solves the system

$$\mathbf{A}\mathbf{x} = \mathbf{b} \quad (\text{C.41})$$

in a least squares sense. Alternatively, we may be given i of smaller sets of equations of the form

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

and again asked to solve for \mathbf{x} . In this latter case, we form the compound matrix $\mathbf{A} = [\mathbf{A}_1^T, \mathbf{A}_2^T \dots \mathbf{A}_I^T]^T$ and compound vector $\mathbf{b} = [\mathbf{b}_1^T, \mathbf{b}_2^T \dots \mathbf{b}_I^T]^T$, and the problem is the same as in equation C.41.

We may equivalently see the same problem in an explicit least-squares form,

$$\hat{\mathbf{x}} = \underset{\mathbf{x}}{\text{argmin}} \left[(\mathbf{A}\mathbf{x} - \mathbf{b})^T (\mathbf{A}\mathbf{x} - \mathbf{b}) \right]. \quad (\text{C.43})$$

Finally, we may be presented the problem as a sum of smaller terms

$$\hat{\mathbf{x}} = \underset{\mathbf{x}}{\operatorname{argmin}} \left[\sum_{i=1}^I (\mathbf{A}_i \mathbf{x} - \mathbf{b}_i)^T (\mathbf{A}_i \mathbf{x} - \mathbf{b}_i) \right], \quad (\text{C.44})$$

in which case we form compound matrices \mathbf{A} and \mathbf{b} , which changes the problem back to that in equation C.43.

To make progress, we multiply out the terms in equation C.43

$$\begin{aligned} \hat{\mathbf{x}} &= \underset{\mathbf{x}}{\operatorname{argmin}} \left[(\mathbf{A}\mathbf{x} - \mathbf{b})^T (\mathbf{A}\mathbf{x} - \mathbf{b}) \right] . \\ &= \underset{\mathbf{x}}{\operatorname{argmin}} \left[\mathbf{x}^T \mathbf{A}^T \mathbf{A} \mathbf{x} - \mathbf{b}^T \mathbf{A} \mathbf{x} - \mathbf{x}^T \mathbf{A}^T \mathbf{b} + \mathbf{b}^T \mathbf{b} \right] \\ &= \underset{\mathbf{x}}{\operatorname{argmin}} \left[\mathbf{x}^T \mathbf{A}^T \mathbf{A} \mathbf{x} - 2\mathbf{x}^T \mathbf{A}^T \mathbf{b} + \mathbf{b}^T \mathbf{b} \right], \end{aligned} \quad (\text{C.45})$$

where we have combined two terms in the last line by noting that they are both the same: they are transposes of one another, but they are also scalars, so they equal their own transpose. Now we take the derivative with respect to \mathbf{x} and equate the result to zero to give

$$2\mathbf{A}^T \mathbf{A} \mathbf{x} - 2\mathbf{A}^T \mathbf{b} = 0, \quad (\text{C.46})$$

which we can re-arrange to give the standard least squares result

$$\mathbf{x} = (\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \mathbf{b}. \quad (\text{C.47})$$

This result can only be computed if there are at least as many rows in \mathbf{A} as there are unknown values in \mathbf{x} (i.e., if the matrix \mathbf{A} is square or portrait). Otherwise, the matrix $\mathbf{A}^T \mathbf{A}$ will be singular. For implementations in Matlab, it is better to make use of the backslash operator ‘\’ rather than explicitly implement equation C.47.

C.7.2 Principal direction / minimum direction

We define the principal and minimal directions as

$$\begin{aligned} \hat{\mathbf{b}} &= \underset{\mathbf{b}}{\operatorname{argmax}} [\mathbf{A}\mathbf{b}] && \text{subject to } |\mathbf{b}| = 1 \\ \hat{\mathbf{b}} &= \underset{\mathbf{b}}{\operatorname{argmin}} [\mathbf{A}\mathbf{b}] && \text{subject to } |\mathbf{b}| = 1, \end{aligned} \quad (\text{C.48})$$

respectively. This problem has exactly the geometric form of figure C.2. The constraint that $|\mathbf{b}| = 1$ means that \mathbf{b} has to lie on the circle (or sphere or hypersphere in higher dimensions). In the principal direction problem, we are hence seeking the direction that is mapped to the major axis of the resulting ellipse/ellipsoid. In the minimum direction problem, we seek the direction that is mapped to the minor axis of the ellipsoid.

We saw in figure C.4 that it is the matrix \mathbf{V} from the singular value decomposition of \mathbf{A} that controls which direction is mapped to the different axes of the ellipsoid. To solve the principal direction problem, we hence compute the SVD $\mathbf{A} = \mathbf{U}\mathbf{L}\mathbf{V}^T$, and set \mathbf{b} to be the first column of \mathbf{V} . To solve the minimum direction problem, we set \mathbf{b} to be the last column of \mathbf{V} .

C.7.3 Orthogonal Procrustes problem

The orthogonal Procrustes problem is to find the closest linear mapping $\mathbf{\Omega}$ between one set of vectors \mathbf{A} and another \mathbf{B} such that $\mathbf{\Omega}$ is an orthogonal matrix. In layman's terms, we seek the best Euclidean rotation (possibly including mirroring) that maps points \mathbf{A} to points \mathbf{B} .

$$\hat{\mathbf{\Omega}} = \underset{\mathbf{\Omega}}{\operatorname{argmin}} [|\mathbf{\Omega}\mathbf{A} - \mathbf{B}|_F], \quad (\text{C.49})$$

where $|\bullet|_F$ denotes the Frobenius norm of a matrix – the sum of the square of all of the elements. To make progress, we recall that the trace of a matrix is the sum of its diagonal entries and so $|\mathbf{X}|_F = \sqrt{\operatorname{tr}[\mathbf{X}^T\mathbf{X}]}$ which gives the new criterion

$$\begin{aligned} \hat{\mathbf{\Omega}} &= \underset{\mathbf{\Omega}}{\operatorname{argmin}} [\operatorname{tr}[\mathbf{A}^T\mathbf{A}] + \operatorname{tr}[\mathbf{B}^T\mathbf{B}] - 2\operatorname{tr}[\mathbf{A}^T\mathbf{\Omega}^T\mathbf{B}]] \\ &= \underset{\mathbf{\Omega}}{\operatorname{argmax}} [\operatorname{tr}[\mathbf{A}^T\mathbf{\Omega}^T\mathbf{B}]] \\ &= \underset{\mathbf{\Omega}}{\operatorname{argmax}} [\operatorname{tr}[\mathbf{\Omega}^T\mathbf{B}\mathbf{A}^T]], \end{aligned} \quad (\text{C.50})$$

where we have used relation C.15 between the last two lines. We now compute the SVD $\mathbf{B}\mathbf{A}^T = \mathbf{U}\mathbf{L}\mathbf{V}^T$ to get the criterion

$$\begin{aligned} \hat{\mathbf{\Omega}} &= \underset{\mathbf{\Omega}}{\operatorname{argmax}} [\operatorname{tr}[\mathbf{\Omega}^T\mathbf{U}\mathbf{L}\mathbf{V}^T]] \\ &= \underset{\mathbf{\Omega}}{\operatorname{argmax}} [\operatorname{tr}[\mathbf{V}^T\mathbf{\Omega}^T\mathbf{U}\mathbf{L}]], \end{aligned} \quad (\text{C.51})$$

and notice that

$$\operatorname{tr}[\mathbf{V}^T\mathbf{\Omega}^T\mathbf{U}\mathbf{L}] = \operatorname{tr}[\mathbf{Z}\mathbf{L}] = \sum_{i=1}^I z_{ii}l_{ii}, \quad (\text{C.52})$$

where we defined $\mathbf{Z} = \mathbf{V}^T\mathbf{\Omega}^T\mathbf{U}$, and used the fact that the \mathbf{L} is a diagonal matrix, so each entry scales the diagonal of \mathbf{Z} on multiplication.

We note that the matrix \mathbf{Z} is orthogonal (it is the product of three orthogonal matrices). Hence, every value on the diagonal of the orthogonal matrix \mathbf{Z} must be less than or equal to one (the norms of each column are exactly one), and so we maximize the criterion in equation C.52 by choosing $\mathbf{Z} = \mathbf{I}$ when the diagonal

values are equal to one. To achieve this, we set $\mathbf{\Omega}^T = \mathbf{V}\mathbf{U}^T$ so that the overall solution is

$$\hat{\mathbf{\Omega}} = \mathbf{U}\mathbf{V}^T. \quad (\text{C.53})$$

A special case of this problem is to find the closest orthogonal matrix $\mathbf{\Omega}$ to a given square matrix \mathbf{B} in a least squares sense. In other words, we seek to optimize

$$\hat{\mathbf{\Omega}} = \underset{\mathbf{\Omega}}{\operatorname{argmin}} [|\mathbf{\Omega} - \mathbf{B}|_F]. \quad (\text{C.54})$$

This is clearly equivalent to optimizing the criterion in equation C.49 but with $\mathbf{A} = \mathbf{I}$. It follows that the solution can be found by computing the singular value decomposition $\mathbf{B} = \mathbf{U}\mathbf{L}\mathbf{V}^T$ and setting $\mathbf{\Omega} = \mathbf{U}\mathbf{V}^T$.

C.8 Tricks for inverting large matrices

Inversion of a $D \times D$ matrix has a complexity of $\mathcal{O}(D^3)$. In practice, this means it is difficult to invert matrices whose dimension is larger than a few thousand. Fortunately, matrices are often highly structured, and we can exploit that structure using a number of tricks to speed up the process.

C.8.1 Diagonal and block-diagonal matrices

Diagonal matrices can be inverted by forming a new diagonal matrix, where the values on the diagonal are reciprocal of the original values. Block diagonal matrices are matrices of the form

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_1 & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \mathbf{A}_2 & \dots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \dots & \mathbf{A}_N \end{bmatrix}. \quad (\text{C.55})$$

The inverse of a block-diagonal matrix can be computed by taking the inverse of each block separately so that

$$\mathbf{A}^{-1} = \begin{bmatrix} \mathbf{A}_1^{-1} & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \mathbf{A}_2^{-1} & \dots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \dots & \mathbf{A}_N^{-1} \end{bmatrix}. \quad (\text{C.56})$$

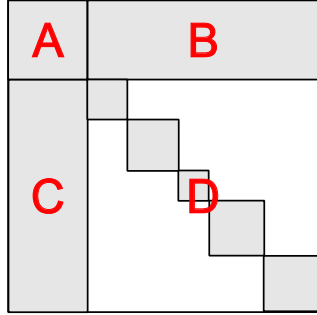


Figure C.5 Inversion relation #1. Gray regions indicate parts of matrix with non-zero values, white regions represent zeros. This relation is suited to the case where the matrix can be divided into four sub-matrices **A**, **B**, **C**, **D** and the bottom right block is easy to invert (e.g., diagonal, block diagonal or structured in another way that means that inversion is efficient). After applying this relation, the remaining inverse is the size of sub-matrix **A**.

C.8.2 Inversion relation #1: Schur complement identity

The inverse of a matrix with sub-blocks **A**, **B**, **C**, and **D** in the top-left, top right, bottom-left, and bottom right positions, respectively, can easily be shown to be

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{bmatrix}^{-1} = \begin{bmatrix} (\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C})^{-1} & -(\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C})^{-1}\mathbf{B}\mathbf{D}^{-1} \\ -\mathbf{D}^{-1}\mathbf{C}(\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C})^{-1} & \mathbf{D}^{-1} + \mathbf{D}^{-1}\mathbf{C}(\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C})^{-1}\mathbf{B}\mathbf{D}^{-1} \end{bmatrix}, \quad (\text{C.57})$$

by multiplying the original matrix with the right hand side and showing that the result is the identity matrix.

This result is extremely useful when the matrix **D** is diagonal or block-diagonal (figure C.5). In this circumstance, \mathbf{D}^{-1} is fast to compute, and the remaining inverse quantity $(\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C})^{-1}$ is much smaller and easier to invert than the original matrix. The quantity $\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C}$ is known as the Schur complement.

C.8.3 Inversion relation #2

Consider the $d \times d$ matrix **A**, the $k \times k$ matrix **C** and the $k \times d$ matrix **B** where **A** and **C** are symmetric, positive definite matrices. The following equality holds:

$$(\mathbf{A}^{-1} + \mathbf{B}^T \mathbf{C}^{-1} \mathbf{B})^{-1} \mathbf{B}^T \mathbf{C}^{-1} = \mathbf{A} \mathbf{B}^T (\mathbf{B} \mathbf{A} \mathbf{B}^T + \mathbf{C})^{-1}. \quad (\text{C.58})$$

Proof:

$$\begin{aligned} \mathbf{B}^T \mathbf{C}^{-1} \mathbf{B} \mathbf{A} \mathbf{B}^T + \mathbf{B}^T &= \mathbf{B}^T + \mathbf{B}^T \mathbf{C}^{-1} \mathbf{B} \mathbf{A} \mathbf{B}^T \\ \mathbf{B}^T \mathbf{C}^{-1} (\mathbf{B} \mathbf{A} \mathbf{B}^T + \mathbf{C}) &= (\mathbf{A}^{-1} + \mathbf{B}^T \mathbf{C}^{-1} \mathbf{B}) \mathbf{A} \mathbf{B}^T. \end{aligned} \quad (\text{C.59})$$

Taking the inverse of both sides we get

$$(\mathbf{A}^{-1} + \mathbf{B}^T \mathbf{C}^{-1} \mathbf{B})^{-1} \mathbf{B}^T \mathbf{C}^{-1} = \mathbf{A} \mathbf{B}^T (\mathbf{B} \mathbf{A} \mathbf{B}^T + \mathbf{C})^{-1}, \quad (\text{C.60})$$

as required.

This relation is very useful when \mathbf{B} is a landscape matrix with many more columns C than rows R . On the left-hand side, the term that we must invert is of size $C \times C$, which might be very costly. However, on the right-hand side, the inversion is only of size $R \times R$, which might be considerably more efficient.

C.8.4 Inversion relation #3: Sherman-Morrison-Woodbury

Consider the $d \times d$ matrix \mathbf{A} , the $k \times k$ matrix \mathbf{C} and the $k \times d$ matrix \mathbf{B} where \mathbf{A} and \mathbf{C} are symmetric, positive definite matrices. The following equality holds:

$$(\mathbf{A}^{-1} + \mathbf{B}^T \mathbf{C}^{-1} \mathbf{B})^{-1} = \mathbf{A} - \mathbf{A} \mathbf{B}^T (\mathbf{B} \mathbf{A} \mathbf{B}^T + \mathbf{C})^{-1} \mathbf{B} \mathbf{A}. \quad (\text{C.61})$$

This is sometimes known as the *matrix inversion lemma*.

Proof:

$$\begin{aligned} (\mathbf{A}^{-1} + \mathbf{B}^T \mathbf{C}^{-1} \mathbf{B})^{-1} &= (\mathbf{A}^{-1} + \mathbf{B}^T \mathbf{C}^{-1} \mathbf{B})^{-1} (\mathbf{I} + \mathbf{B}^T \mathbf{C}^{-1} \mathbf{B} \mathbf{A} - \mathbf{B}^T \mathbf{C}^{-1} \mathbf{B} \mathbf{A}) \\ &= (\mathbf{A}^{-1} + \mathbf{B}^T \mathbf{C}^{-1} \mathbf{B})^{-1} ((\mathbf{A}^{-1} + \mathbf{B}^T \mathbf{C}^{-1} \mathbf{B}) \mathbf{A} - \mathbf{B}^T \mathbf{C}^{-1} \mathbf{B} \mathbf{A}) \\ &= \mathbf{A} - (\mathbf{A}^{-1} + \mathbf{B}^T \mathbf{C}^{-1} \mathbf{B})^{-1} \mathbf{B}^T \mathbf{C}^{-1} \mathbf{B} \mathbf{A}. \end{aligned} \quad (\text{C.62})$$

Now, applying inversion relation #2 to the term in brackets:

$$\begin{aligned} (\mathbf{A}^{-1} + \mathbf{B}^T \mathbf{C}^{-1} \mathbf{B})^{-1} &= \mathbf{A} - (\mathbf{A}^{-1} + \mathbf{B}^T \mathbf{C}^{-1} \mathbf{B})^{-1} \mathbf{B}^T \mathbf{C}^{-1} \mathbf{B} \mathbf{A} \\ &= \mathbf{A} - \mathbf{A} \mathbf{B}^T (\mathbf{B} \mathbf{A} \mathbf{B}^T + \mathbf{C})^{-1} \mathbf{B} \mathbf{A}, \end{aligned} \quad (\text{C.63})$$

as required.

C.8.5 Matrix determinant lemma

The matrices that we need to invert are often the covariances in the normal distribution. When this is the case we sometimes also need to compute the determinant of the same matrix and this may be prohibitively expensive. Fortunately, there is a direct analogy of the matrix inversion lemma for determinants which can reduce the cost when the covariance is structured.

Consider the $d \times d$ matrix \mathbf{A} , the $k \times k$ matrix \mathbf{C} and the $k \times d$ matrix \mathbf{B} where \mathbf{A} and \mathbf{C} are symmetric, positive definite covariance matrices. The following equality holds:

$$|\mathbf{A}^{-1} + \mathbf{B}^T \mathbf{C}^{-1} \mathbf{B}| = |\mathbf{I} + \mathbf{B} \mathbf{A} \mathbf{B}^T| |\mathbf{C}|^{-1} |\mathbf{A}|^{-1}. \quad (\text{C.64})$$

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