Chapter 1

Image Restoration

ch, restore

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1.1 Introduction (s,res,intro)

Although this book emphasizes tomographic **image reconstruction** problems, many of the concepts apply to the related inverse problem known as **image restoration**. The physical models used in basic image restoration problems are often simpler than those of realistic tomographic reconstruction problems, so image restoration problems provide a convenient framework in which to describe many of the principles of **image recovery** problems¹ in general, both restoration and reconstruction problems². This *chapter* uses the context of image restoration problems to provide an overview of the concepts that will follow later in the book. By no means is this an exhaustive treatment of image restoration; the focus is on principles that are common to both restoration and reconstruction. Readers familiar with statistical image restoration methods could simply skim this chapter for the notation conventions. For further reading, see [2–6].

In 2D image restoration problems, we are given a blurry, noisy image

$$\{g[m,n] \in \mathbb{R} : m = 0, \dots, M-1, \ n = 0, \dots, N-1\}$$
(1.1.1)

of some object or scene, recorded, for example, by a camera with a digital detector such as a **CCD array** [7, 8]. Restoration of astronomical images from the Hubble Space Telescope is a famous example of such a problem [9]. Our

¹There is not universal terminology for image recovery problems. Typically **image reconstruction** means forming an image from measured data that is not interpretable directly as an image, such as a **sinogram** in tomography. In contrast, in **image restoration** problems one begins with an image (usually noisy and blurry) and tries to improve it. A special case is **image denoising** where one tries to reduce noise without considering blur. We use **image recovery** to encompass all such problems.

 $^{^{2}}$ In the context of medical imaging, iterative methods for image restoration were applied as far back as 1967 [1].

goal is to use the measured image to form an estimate of the underlying "true" object, *i.e.*, to eliminate or reduce the blur and the noise. We focus on 2D problems, but the concepts generalize readily to 3D restoration problems like confocal microscopy [10] and to problems with multiple views of the same object [11–14].

Fig. 1.1.1 illustrates image restoration using a method described in §1.8.2.





Figure 1.1.1: The left image was degraded by a 11×11 uniform blur b[m, n] and additive gaussian noise corresponding to 60 dB blurred signal-to-noise ratio (**BSNR**). The right image illustrates deblurring using the method in §1.8.2.

To proceed, we must define the restoration goal more precisely. An ambitious goal would be to try to reconstruct the image that would be recorded by an imaging device with perfect spatial resolution, sufficiently large field of view, arbitrary dynamic range, and no measurement errors (noiseless). Practical formulations are usually less ambitious, as described next.

1.2 Conventional discrete measurement model

The simplest formulations of image restoration problems assume that the object to be recovered is also a discrete-space array with the same domain as g[m, n]. In other words, we wish to estimate the **latent image** (unknown object)

$$\{f[m,n] \in \mathbb{R} : m = 0, \dots, M-1, \ n = 0, \dots, N-1\}$$
(1.2.1)

from the measurements $\{g[m, n]\}$. The first step in formulating any inverse problem is to define a system model that relates the unknown quantities to the observed measurements. In the signal processing literature, this is known as the **input-output relationship** of the system. In the inverse problems field, this is called the **forward model** for the problem. Several of the subsequent chapters focus on system models for tomographic systems.

For image restoration, the simplest model is to assume that the imaging system is **linear** and **shift-invariant**. The input-output relationship of any linear shift-invariant (LSI) system can be represented by a **convolution** operation. For a discrete-space LSI system, the convolution sum is³

$$\bar{g}[m,n] = b[m,n] ** f[m,n] \triangleq \sum_{k=0}^{M-1} \sum_{l=0}^{N-1} b[m-k,n-l] f[k,l],$$
(1.2.2)

where b[m, n] denotes the **impulse response** of the system, or specifically the **point spread function** (**PSF**) in the context of imaging problems. Typically b[m, n] causes *blur*.

The convolution model (1.2.2) by itself is incomplete because any real imaging system has measurement errors, known as "noise." (This terminology comes from the influence of audio signals in the signal processing field). Several subsequent chapters describe statistical models for tomographic measurements. For image restoration, the simplest model assumes that the measurement noise $\varepsilon[m, n]$ is additive:

$$g[m,n] = b[m,n] ** f[m,n] + \varepsilon[m,n], \qquad m = 0, \dots, M-1, \ n = 0, \dots, N-1.$$
(1.2.3)

Often it is assumed that the noise is zero mean and has a gaussian distribution. Fig. 1.2 illustrates this model.

³The notation $\bar{g}[m,n] = (b * * f)[m,n]$ would be more precise. The standard definition of the 2D convolution sum is $(b * * f)[m,n] = \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} b[m-k,n-l] f[k,l]$. For now, we treat $f[\cdot, \cdot]$ as being zero for arguments outside its domain (1.2.1). We revisit this assumption in §1.4.



Figure 1.2.1: Graphical illustration of the imaging model (1.2.3) for the extended end conditions of §1.4.1.2.

With the statistical model (1.2.3) in hand, we can state that the goal of image restoration is to recover $\{f[m,n]\}$ from $\{g[m,n]\}$, using knowledge of the PSF b[m,n] and a statistical model for the noise $\varepsilon[m,n]$. A challenging variation of this problem is **blind restoration** in which the PSF b[m,n] is also unknown or partially unknown, *e.g.*, [15–37]. This problem is particularly interesting when given multiple images with different blurs [12, 28, 38–43].

Although (1.2.3) is the classical model for image restoration that has been the focus of numerous publications, there are very few, if any, realistic problems that exactly match the underlying assumptions! The unknown object is rarely a discrete-space function, imaging systems are rarely perfectly shift invariant (due to problems like optical aberrations), and in optical imaging the noise is rarely exactly gaussian due to the quantum effects of photons. Furthermore, digital detectors always quantize the measurements. There are also subtle effects at the borders of the field of view that require consideration.

The mismatch between the classical model and physical reality is not unique to image restoration problems; many tomography papers have also been based on over-simplified models. Simplified models are certainly very important for developing intuition and, in many cases, for finding fast (albeit approximate) algorithms. But one of the goals of subsequent chapters is to describe reasonably complete models for tomographic systems because one of the most important benefits of statistical methods for image reconstruction is that they can incorporate realistic models, whereas analytical reconstruction methods usually are limited to relatively simplified models.

As a preview of the types of system models that are described in subsequent chapters, we consider next a somewhat more realistic model for many image restoration problems, and attempt to relate it to (1.2.3).

1.3 Continuous-discrete model (s,res,cd)

Although no physical system can be perfectly linear over an arbitrary dynamic range, practical systems are usually designed to operate within the linear range of the system components. So the linearity assumption that underlies (1.2.2) is often reasonable. However, in most image restoration problems the (unknown) "true object" is a function of continuous arguments, called a **continuous-space function**, *e.g.*, $\{f(x, y) : x, y \in \mathbb{R}\}$, so using a discrete-space object and PSF in (1.2.2) is a simplification. Compared to (1.2.2), a more realistic measurement model for image restoration problems is the following [44]:

$$g[m,n] = \overline{g}[m,n] + \varepsilon[m,n], \quad \overline{g}[m,n] = \iint b(m,n;x,y) f(x,y) \,\mathrm{d}x \,\mathrm{d}y, \tag{1.3.1}$$

where b(m, n; x, y) denotes the contribution that an impulse object located at (x, y) would make to the expected value of g[m, n]. The function b(m, n; x, y), combined with the assumption of linearity, completely describes the non-statistical aspects of the imaging system, so we refer to b(m, n; x, y) as the system model.

The model (1.3.1) is known as a **continuous to discrete mapping**. With this model, we could pose the problem as one of estimating f given $\{g[m, n]\}$. This problem is the epitome of under-determined; there are uncountably many f that agree exactly with the measurements g[m, n], even for noiseless data where $\varepsilon[m, n] = 0$.

1.3.1 Ill-posed problems

Trying to reconstruct f from $\{g[m, n]\}$ is an example of an **ill-posed problem**. Problems are called **well-posed** in the sense of Hadamard [45, p. 63] when a solution exists that is unique and stable (continuous) with respect to the data. Otherwise a problem is called ill-posed.

In imaging problems with a underlying continuous-space object f but a finite number of measurements, nonuniqueness is the principal challenge. Clearly we must impose some type of prior knowledge (or prior assumptions) about f to proceed.

Most methods in the literature avoid the complications of the continuous-discrete model (1.3.1) by adopting either a continuous-continuous formulation, or, more often, the discrete-discrete formulation (1.2.2). An example of a continuous-continuous model is

$$g(x,y) = b(x,y) * f(x,y) + \varepsilon(x,y), \qquad (1.3.2)$$

where b(x, y) denotes a continuous-space PSF and $\varepsilon(x, y)$ denotes a **random noise process**. One can derive estimators $\hat{f}(x, y)$ in terms of the "given" continuous-space image g(x, y) in this framework. One simple example is the continuous-space Wiener filter (*cf.* the discrete-space version in (1.7.11)). Another broader family of methods uses partial differential equation (PDE) methods to address (1.3.2) [46]. Of course in practice we never have a continuous-space g(x, y) available in a computer, so one must somehow discretize any such solution expressions to implement a practical estimator in terms of g[m, n].

Although subsequent sections focus on the discrete-discrete formulation (1.2.3), for completeness we mention one particular approach that is formulated directly from the continuous-discrete model (1.3.1).

1.3.2 Minimum norm estimate

Even if there were no noise in (1.3.1), *i.e.*, if $\varepsilon[m, n] = 0$, there would still be many images f that satisfy exactly the equalities in (1.3.1). One way to pick a solution from this infinite set is to choose the solution with minimum \mathcal{L}_2 norm (*i.e.*, minimum energy in signal processing terminology). By the projection theorem (an important result from functional analysis [47, p. 51]), a unique solution with minimum norm exists. It can be expressed as

$$\hat{f} = \underset{f \in \mathcal{C}(g)}{\operatorname{arg\,min}} \iint |f(x,y)|^2 \, \mathrm{d}x \, \mathrm{d}y, \tag{1.3.3}$$

where C(q) denotes the following **convex set** (see §29.9.1):

$$\mathcal{C}(g) \triangleq \left\{ f : \iint b(m,n;x,y) f(x,y) \, \mathrm{d}x \, \mathrm{d}y = g[m,n], \quad \forall m,n \right\}.$$
(1.3.4)

One can calculate the minimum norm solution using a certain **singular value decomposition** (**SVD**) [48]. The resulting solution has the form

$$\hat{f}(x,y) = \sum_{m,n} c_{m,n} \ b(m,n;x,y)$$
(1.3.5)

for some coefficients $\{c_{m,n}\}$ that depend on the data $\{g[m,n]\}$ and on the system model $b(\cdot)$. This minimum-norm solution is convenient for analysis, but rarely is there any physical reason why real objects should be of minimum norm, so this criterion for picking one of many solutions is just as *ad hoc* as any alternative. (In fact, one could replace the usual norm in (1.3.3) with many alternative norms (or semi-norms) [49–51].) Furthermore, enforcing strict data consistency in (1.3.4) essentially means that noise is ignored.

The subject of **regularization** is closely related to this problem of choosing from an infinite collection of solutions, and is a major focus of Chapter 2 and other portions of several chapters of this book.

1.3.3 Object models

The minimum norm approach is one way to impose (fairly weak) prior information to select a solution. A different approach would be to assume that the unknown object f lies in a **subspace** of \mathcal{L}_2 , *i.e.*, a linear combination of some basis functions. This type of assumption serves to bridge the continuous-discrete model (1.3.1) with the discrete-discrete model (1.2.2). Typically the basis functions are just equally spaced versions of a common kernel $\beta_0(x, y)$ as used in the following representation:

$$f(x,y) = \sum_{m,n} f[m,n] \beta_0(x - m\Delta_x, y - n\Delta_y), \qquad (1.3.6)$$

where \triangle_x and \triangle_y denote the spacing of the basis functions. Under such a model, the image restoration goal is to estimate the coefficients $\{f[m,n]\}$ from the measurements $\{g[m,n]\}$.

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For example, a common assumption in signal processing is that f is a **band-limited** function. If so, then by the 2D **sampling theorem** [52, p. 238] there exist sample distances \triangle_x and \triangle_y for which (1.3.6) is exact with an appropriate sinc kernel:

$$\beta_0(x, y) = \operatorname{sinc}_2(x/\Delta_x, y/\Delta_y)$$

$$\operatorname{sinc}_2(x, y) \triangleq \operatorname{sinc}(x) \operatorname{sinc}(y)$$

$$\operatorname{sinc}(x) \triangleq \begin{cases} \frac{\sin(\pi x)}{\pi x}, & x \neq 0\\ 1, & x = 0. \end{cases}$$
(1.3.7)

In general, however, (1.3.6) is merely an approximation.

Another common choice is to use 2D rectangular functions as basis functions: $\beta_0(x, y) = \text{rect}_2(x/\Delta_x, y/\Delta_y)$, which correspond to rectangular (or square in the usual case when $\Delta_x = \Delta_y$) pixels of uniform value f[m, n].

Often the basis functions satisfy the interpolation property

$$\beta_0(m \triangle_{\mathbf{x}}, n \triangle_{\mathbf{y}}) = \begin{cases} 1, & n = m = 0\\ 0 & \forall m, n \in \mathbb{Z} - \{0, 0\}, \end{cases}$$

in which case $f[m,n] = f(m \triangle_x, n \triangle_y)$. The sinc and rect examples both satisfy this property.

Substituting the object model (1.3.6) into the integral in (1.3.1) yields

$$\bar{g}[m,n] = \iint b(m,n;x,y) f(x,y) \, \mathrm{d}x \, \mathrm{d}y$$

$$= \iint b(m,n;x,y) \left[\sum_{k,l} f[k,l] \beta_0(x-k\triangle_x, y-l\triangle_y) \right] \, \mathrm{d}x \, \mathrm{d}y$$

$$= \sum_{k,l} b[m,n;k,l] f[k,l], \qquad (1.3.8)$$

where the "discrete-discrete" impulse response is

$$b[m,n;k,l] \triangleq \iint b(m,n;x,y) \,\beta_0(x-k\Delta_{\mathbf{x}},y-l\Delta_{\mathbf{y}}) \,\mathrm{d}x \,\mathrm{d}y \,. \tag{1.3.9}$$

Suppose we further assume that the imaging system is shift invariant in the following sense:

$$b(m,n;x,y) = b_0(x - m\Delta_x, y - n\Delta_y), \qquad (1.3.10)$$

for some 2D PSF $b_0(x, y)$. An imaging system having a system response that satisfies (1.3.10) has the property that shifting the input object by an integer number of sample distances causes a corresponding shift of the output image. The model (1.3.10) is often a reasonable approximation, with the caveat that (1.3.10) assumes implicitly that the detector sample spacing is matched to the object model. Under this assumption, the discrete-discrete impulse response is also shift invariant:

$$\begin{split} b[m,n;k,l] &= \iint b(m,n;x,y) \,\beta_0(x-k\triangle_{\mathbf{x}},y-l\triangle_{\mathbf{y}}) \,\mathrm{d}x \,\mathrm{d}y \\ &= \iint b_0(x-m\triangle_{\mathbf{x}},y-n\triangle_{\mathbf{y}}) \,\beta_0(x-k\triangle_{\mathbf{x}},y-l\triangle_{\mathbf{y}}) \,\mathrm{d}x \,\mathrm{d}y \\ &= \iint b_0(x-(m-k)\triangle_{\mathbf{x}},y-(m-l)\triangle_{\mathbf{y}}) \,\beta_0(x,y) \,\mathrm{d}x \,\mathrm{d}y \\ &= b[m-k,n-l;0,0], \end{split}$$

assuming appropriate limits for the integrals. With these assumptions, we have

$$\bar{g}[m,n] = \sum_{k,l} b[m-k,n-l;0,0] f[k,l], \qquad (1.3.11)$$

which is equivalent to (1.2.2) except for (nontrivial!) details about the summation limits, as detailed in §1.4. So we have established that there is at least one set of conditions (namely (1.3.6) and (1.3.10)) under which the continuous-discrete model (1.3.1) will (almost) simplify to the discrete-discrete model (1.2.2).

If the true f(x, y) contains sharp edges, then the model (1.3.6) may lead to blurred estimates of those edges. To preserve such edges, it may be desirable to use a basis for f(x, y) that has smaller pixels than the sample spacing of the measurements g[m, n]. This will result in an under-determined problem, but this can be addressed using edgepreserving regularization, as discussed in §1.10. Even if an image is band-limited, using the object model (1.3.6) with the sinc basis (1.3.7) is usually inconvenient for implementation. On the other hand, the expansion (1.3.5) also seems awkward because it is imaging system dependent. Chapter 10 describes various basis functions for representing a continuous object f in terms of a finite set of parameters or expansion coefficients.

1.4 Matrix-vector representations of convolution (s,res,mat1)

The convolution notation (1.2.3) is ubiquitous in signal processing, and corresponding Fourier concepts are commonly expressed in these terms. For example, the very important **convolution property** of the 2D **Fourier transform** can be written:

$$\bar{g}[m,n] = b[m,n] ** f[m,n] \stackrel{\text{DSFT}}{\longleftrightarrow} \bar{G}(\Omega_1,\Omega_2) = B(\Omega_1,\Omega_2) F(\Omega_1,\Omega_2), \tag{1.4.1}$$

where the 2D (discrete space) Fourier transform (DSFT) of b[m, n] is defined by:

$$B(\Omega_1, \Omega_2) = \sum_{m,n} b[m, n] e^{-i(\Omega_1 m + \Omega_2 n)}, \qquad (1.4.2)$$

and Ω_1, Ω_2 denote **digital frequencies** having units radians/sample. However, the convolution notation becomes inconvenient when one wants to relate signal processing concepts to methods from numerical linear algebra or statistics. Convolution is a linear operator, so we can represent the convolution operator using **matrix-vector notation**. Matrixvector notation is also more convenient for describing system models that generalize (1.2.3), such as shift variant imaging systems and tomographic imaging systems. Facility with both signal processing notation and matrix-vector representations is essential for working with image recovery problems, so this section describes in detail how to relate these representations.

1.4.1 1D matrix-vector representations

For simplicity we first consider a 1D version of the signal restoration problem. Consider a 1D convolution relationship for an input signal f[n] as follows:

$$g[n] = \bar{g}[n] + \varepsilon[n], \quad \bar{g}[n] = b[n] * f[n] = \sum_{k} b[n-k] f[k], \quad n = 0, \dots, N-1.$$
(1.4.3)

We want to represent the preceding "DSP-style" formula in the following matrix-vector form

$$\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{\varepsilon}, \tag{1.4.4}$$

where y, ε , and x are column vectors (with y and x possibly having somewhat different lengths), and A is a matrix whose entries depend solely on the values of b[n]. When stored in a computer, the vectors y and x must have finite length, whereas the convolution sum in (1.4.3) above can have arbitrary indices "on paper," even $\sum_{k=-\infty}^{\infty}$, but that is impractical for computation. There are various choices for A depending on how we handle the "end conditions," *i.e.*, depending on how we choose the limits of the summation in (1.4.3). In all cases we form the measurement vector y from the measurements g[n] in the obvious way:

$$\boldsymbol{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix} = \begin{bmatrix} g[0] \\ \vdots \\ g[N-1] \end{bmatrix}, \qquad (1.4.5)$$

i.e., $y_i = g[i-1]$. For consistency with matrix algebra conventions, the vector index *i* starts at 1, whereas for consistency with signal processing (and ANSI C) conventions, the sample index *n* starts at 0. We define the noise vector $\boldsymbol{\varepsilon}$ similarly.

For vectorizing the measurements, (1.4.5) is the only natural choice because N is a particular value depending on the measurement system. However, there is somewhat more flexibility when we choose A and x, because these are

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merely models. For concreteness, we illustrate the various choices using a hypothetical 1D imaging system that has the following 3-point impulse response:

$$b[n] = b[-1]\,\delta[n+1] + b[0]\,\delta[n] + b[1]\,\delta[n-1],$$

where the Kronecker impulse function is denoted

-

$$\delta[n] \triangleq \begin{cases} 1, & n = 0\\ 0, & \text{otherwise.} \end{cases}$$
(1.4.6)

For each of the end conditions described below, Fig. 1.4.1 gives an example of the corresponding matrix A.

1.4.1.1 Zero end conditions

The simplest model is to assume that f[n] is zero for n < 0 and for $n \ge N$, and to use $\sum_{k=0}^{N-1}$ in the convolution sum (1.4.3). If this "zero end condition" (also known as a **Dirichlet boundary condition**) assumption is appropriate, then natural choices for x and A are as follows:

$$\boldsymbol{A} = \begin{bmatrix} b[0] & b[-1] & 0 & \cdots & 0 & 0 & 0\\ b[1] & b[0] & b[-1] & 0 & \cdots & 0 & 0\\ 0 & b[1] & b[0] & b[-1] & 0 & \cdots & 0\\ & & & \ddots & & & \\ 0 & \cdots & 0 & b[1] & b[0] & b[-1] & 0\\ 0 & 0 & \cdots & 0 & b[1] & b[0] & b[-1]\\ 0 & 0 & 0 & \cdots & 0 & b[1] & b[0] \end{bmatrix}, \qquad \boldsymbol{x} = \begin{bmatrix} f[0] \\ \vdots \\ f[N-1] \end{bmatrix}.$$
(1.4.7)

This $N \times N$ matrix A is **Toeplitz** (constant along the diagonals), and there are reasonably fast algorithms for manipulating (*e.g.*, inverting) such matrices [53, 54]. In this 1D case, the elements $\{a_{ij}\}$ of A are related to a general impulse response function b[n] as follows:

$$a_{ij} = b[i-j], \qquad i, j = 1, \dots, N.$$
 (1.4.8)

However, in the shift-invariant case, relatively rarely does one actually implement A literally as a matrix. Computing Ax yields the same result as convolving b[n] and f[n], so usually one would simply pass the elements of b[n] and f[n] to a convolution routine. So for shift-invariant problems, the matrix-vector representation is more for convenience of mathematical *analysis* than for *implementation*. On the other hand, for shift-variant problems, storing A as a matrix is often appropriate, although a sparse matrix representation [55, p. 78] is usually most efficient due to the small percentage of nonzero elements in A when b[n] has just a few non-zero values.

1.4.1.2 Extended end conditions

s, res, mat1, extend

In many situations, *e.g.*, optical imaging, the measurements are influenced by a larger scene than the field of view of the aperture due to the spreading caused by the imaging system PSF. In such cases, assuming zero end conditions can be unrealistic and one may need to allow for objects of extended size (relative to the measurements) in the system model⁴ [57–61]. With regularization (discussed later) or constraints, partial recovery of an extended object can be possible, *i.e.*, the object vector x can have somewhat more elements than the measurement vector y. In such cases, natural choices for x and A include the following:

$$\boldsymbol{A} = \begin{bmatrix} b[1] & b[0] & b[-1] & 0 & \cdots & 0 & 0\\ 0 & b[1] & b[0] & b[-1] & 0 & \cdots & 0\\ & \ddots & \ddots & \ddots & & \\ 0 & 0 & \cdots & 0 & b[1] & b[0] & b[-1] \end{bmatrix}, \qquad \boldsymbol{x} = \begin{bmatrix} f[-1] \\ f[0] \\ \vdots \\ f[N-1] \\ f[N] \end{bmatrix}.$$
(1.4.9)

Here A is a $N \times (N + L - 1)$ rectangular matrix where L is the length of the impulse response (L = 3 for this particular b[n]).

In my view, these **extended end conditions** are more realistic that the other end conditions for most restoration problems and should be used in practice whenever feasible. However, often engineers like to "cut corners" to save

e,kronecker

e,res,aij,bn

⁴This problem is so important in helical cone-beam tomography that it has been dubbed the "long object problem" [56].

computation. The next sections describe the "replicated," "mirror" and "periodic" end conditions that are often used in practice, essentially as approximations to the extended end conditions.

Mat If b is the row vector $[b[-1] \ b[0] \ b[1]]$, the MATLAB command A = convmtx(fliplr(b), N) generates this A. Again, the matrix representation of convolution is more useful for analysis than for computation. Mat This model is related to MATLAB's wall is dention for the 2D convolution routine conve?

Mat This model is related to MATLAB's valid option for the 2D convolution routine conv2.

1.4.1.3 Replicated end conditions

If the zero end conditions are unrealistic but the extended end conditions are considered infeasible, an alternative is to assume that the signal beyond the field of view is similar to the signal at the borders of the field of view, *i.e.*, f[n] = f[0] for n < 0 and f[n] = f[N-1] for $n \ge N$ in 1D. For the case L = 3 this assumption corresponds to models where f[-1] = f[0] and f[N] = f[N-1]. In matrix-vector form this leads to the same N-point x as in (1.4.7), but where A has the following $N \times N$ square form:

$$\boldsymbol{A} = \begin{bmatrix} b[0] + b[1] & b[-1] & 0 & \cdots & 0 & 0\\ b[1] & b[0] & b[-1] & 0 & \cdots & 0\\ & & \ddots & & & \\ 0 & \cdots & 0 & b[1] & b[0] & b[-1]\\ 0 & 0 & \cdots & 0 & b[1] & b[0] + b[-1] \end{bmatrix}.$$
(1.4.10)

All rows of this A have the same cumulative sum; this property is desirable because if x is a uniform image then so is Ax.

1.4.1.4 Mirror end conditions

A variation on the previous approach is to use **mirror end conditions** [62, Box 2], also known as **reflective boundary** conditions or Neumann boundary conditions [63], where we assume that f[-n] = f[n] and f[N-1+n] = f[N-1-n] for n = 0, ..., N-1. Specifying the corresponding A is left to Problem 1.8.

1.4.1.5 Periodic end conditions

Another choice for end conditions in (1.4.3) is to assume that f[n] is *N*-periodic, *i.e.*, that⁵ $f[n] = f[n \mod N]$. Periodic end conditions rarely (if ever) hold exactly in practical imaging systems, but are a very useful approximation for *analyzing* algorithms in the frequency-domain, as described in §1.4.3.1 below. Under this assumption, one can show (Problem 1.3) that the linear convolution (1.4.3) becomes a *N*-point circular convolution:

$$\bar{g}[n] = \tilde{b}[n] \circledast_N f[n] \triangleq \sum_{k=0}^{N-1} \tilde{b}[(n-k) \mod N] f[k], \quad n = 0, \dots, N-1,$$
(1.4.11)

where the periodic superposition of b[n] is defined by

$$\tilde{b}[n] \triangleq \sum_{l} b[n-lN] \,. \tag{1.4.12}$$

Usually we assume that the blur kernel b[n] is zero for $|n| \ge N$, in which case (1.4.12) simplifies to

 $\tilde{b}[n] = b[n] + b[n - N], \quad n = 0, \dots, N - 1.$

For the circular convolution model, the matrix-vector representation uses the same x as in (1.4.7), but the $N \times N$ system matrix A becomes

$$\boldsymbol{A} = \begin{bmatrix} \tilde{b}[0] & \tilde{b}[N-1] & \tilde{b}[N-2] & \cdots & \tilde{b}[2] & \tilde{b}[1] \\ \tilde{b}[1] & \tilde{b}[0] & \tilde{b}[N-1] & \tilde{b}[N-2] & \cdots & \tilde{b}[2] \\ & \ddots & & & \\ \tilde{b}[N-1] & \tilde{b}[N-2] & \tilde{b}[N-3] & \cdots & \tilde{b}[1] & \tilde{b}[0] \end{bmatrix}.$$
(1.4.13)

⁵Here, the modulo operator is defined by $n \mod N = n - N \lfloor n/N \rfloor$, where the floor function $\lfloor t \rfloor$ denotes the largest integer no greater than t. See §29.12.

Zero:	$\left[\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Extended: $ \begin{bmatrix} 1 & 4 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 4 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 4 & 2 & 0 & 0 \\ 0 & 0 & 0 & 1 & 4 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 4 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 4 & 2 \end{aligned} $
Replicated:	$\left[\begin{array}{ccccccccccc} 5 & 2 & 0 & 0 & 0 & 0 \\ 1 & 4 & 2 & 0 & 0 & 0 \\ 0 & 1 & 4 & 2 & 0 & 0 \\ 0 & 0 & 1 & 4 & 2 & 0 \\ 0 & 0 & 0 & 1 & 4 & 2 \\ 0 & 0 & 0 & 0 & 1 & 6 \end{array}\right]$	Mirror: $ \begin{bmatrix} 4 & 3 & 0 & 0 & 0 & 0 \\ 1 & 4 & 2 & 0 & 0 & 0 \\ 0 & 1 & 4 & 2 & 0 & 0 \\ 0 & 0 & 1 & 4 & 2 & 0 \\ 0 & 0 & 0 & 1 & 4 & 2 \\ 0 & 0 & 0 & 0 & 3 & 4 \end{bmatrix} $
	Periodic/circulant:	$\left[\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$

Figure 1.4.1: Concrete examples of system matrices A for 1D convolution with various end conditions, for $b[n] = \{2 \ \underline{4} \ 1\} = 2 \ \delta[n+1] + 4 \ \delta[n] + \delta[n-1]$, for the case N = 6.

In this case $a_{ij} = \tilde{b}[(i-j) \mod N]$. This matrix A is called **circulant**, and can be considered to be an approximation to the Toeplitz form (1.4.7).

See [64–66] for discussion of restoration using **anti-reflective boundary conditions**, and [67] for further alternatives.

s, res, mat2 1.4.2 2D matrix-vector representations (s, res, mat2)

For 2D (and higher dimensional) problems, the same general principles apply when representing convolutions with matrix-vector notation. The expressions relating the convolution form to the matrix-vector representation are messier, but, when expressed in matrix-vector form, both the 1D and 2D cases look like (1.4.4).

1.4.2.1 Lexicographic ordering

The first step is to represent a finite-sized image g[m, n] using a "long" vector via a **lexicographic order**. Specifically, if g[m, n] has the $M \times N$ domain defined in (1.1.1), then the corresponding vector \boldsymbol{y} is of length MN and the *i*th element of \boldsymbol{y} is given by

$$y_i = g[m(i), n(i)], \qquad i = 1, \dots, MN,$$
(1.4.14)

where vector index *i* maps to pixel coordinates [m(i), n(i)] as follows:

$$m(i) \triangleq (i-1) \mod M$$
$$n(i) \triangleq \left\lfloor \frac{i-1}{M} \right\rfloor.$$
(1.4.15)

Again the index *i* starts at 1, for consistency with matrix algebra, and the indices [m, n] start at 0, for consistency with signal processing conventions. Spatial index [m, n] corresponds to i = 1 + m + nM, *i.e.*,

$$g[m,n] = y_i \Big|_{i=1+m+nM}.$$
(1.4.16)

The following figure summarizes the relationship between the vector y and the 2D image g[m, n]. One can define

e,res,mat2,mn

e, res, mat2, i=1+m+nM



Figure 1.4.2: Illustration of system matrices A for 1D blur with different end conditions, for N = 9. The colors of the values used in A match those shown in the PSF b[n].

a vec operator, vec : $\mathbb{R}^{M \times N} \to \mathbb{R}^{MN}$, such that y = vec(g). This operation is called vectorization.

$y_1 = g[0,0]$	$y_2 = g[1,0]$		$y_M = g[M-1,0]$	
$y_{M+1} = g[0,1]$	$y_{M+2} = g[1,1]$		$y_{2M} = g[M-1,1]$	$\rightarrow n$
		:		$\begin{pmatrix} * \\ n \end{pmatrix}$
$u_{M(N-1)+1} = q[0, N-1]$	$u_{M(N-1)+2} = a[1, N-1]$	•	$u_{MN} = a[M-1, N-1]$	10

Mat MATLAB's reshape, colon, (:), sub2ind, and ind2sub routines are useful for such conversions.

We define vector $\boldsymbol{x} = \text{vec}(f)$ in terms of the **latent image** f[m, n] in a manner similar to (1.4.14). The length of \boldsymbol{x} depends on the boundary conditions used. For zero or periodic or mirror boundary conditions, \boldsymbol{x} is a vector of length MN where $x_j = f[m(j), n(j)]$ where $[m(\cdot), n(\cdot)]$ were defined in (1.4.15). For extended end conditions the vector \boldsymbol{x} is longer.

Using such lexicographic ordering, by linearity we can always write the 2D convolution expression (1.2.2), or the more general **superposition sum** (1.3.8), in the matrix-vector form (1.4.4), *i.e.*,

$$y = Ax + \varepsilon$$
.

The exact form of A depends again on the chosen end conditions.

1.4.2.2 Zero-end conditions

Consider the general discrete-space superposition sum

$$\bar{g}[m,n] = \sum_{k,l} b[m,n;k,l] f[k,l], \qquad \begin{array}{l} m = 0, \dots, M-1 \\ n = 0, \dots, N-1. \end{array}$$
(1.4.17)

This sum characterizes the **input-output relationship** of any 2D discrete-space linear system, and this generality is needed for shift-variant systems. If one uses the end conditions that f[m, n] is zero outside the domain m=0,...,M-1, n=0,...,N-1, then the corresponding system matrix A has size $MN \times MN$ and has entries

$$a_{ij} = b[m(i), n(i); m(j), n(j)],$$
(1.4.18)

fig res matl

where $m(\cdot)$ and $n(\cdot)$ were defined in (1.4.15). Expressed another way:

$$a_{1+m+nM, 1+m+nM} = b[m, n; k, l]$$

for $m, k = 0, \ldots, M - 1$ and $n, l = 0, \ldots, N - 1$. Any such matrix A has the following block matrix form:

$$\boldsymbol{A} = \begin{bmatrix} \boldsymbol{A}_{0,0} & \cdots & \boldsymbol{A}_{0,N-1} \\ \vdots & \ddots & \vdots \\ \boldsymbol{A}_{N-1,0} & \cdots & \boldsymbol{A}_{N-1,N-1} \end{bmatrix}, \qquad (1.4.19)^{\text{e,res,mat2,1}}$$

where the $M \times M$ submatrix A_{nl} describes how the *l*th row of the input image contributes to the *n*th row of the output image and has elements

$$\left[\boldsymbol{A}_{nl}\right]_{mk} = b[m, n; k, l] \,.$$

See Fig. 1.4.3 for an example.

Other end conditions have similar expressions (see Problem 1.9) with different values for the elements of A corresponding to pixels at the borders of the image. In general, we can always write (1.4.17) as $\bar{y} = Ax$ using such an A.

See [68] for statistical methods for dealing with boundary artifacts that arise from end condition choices. Mat MATLAB's convmtx2 uses zero-end conditions but produces a sparse matrix that has more rows than columns.

1.4.2.3 Shift-invariant 2D blur and Toeplitz matrices

If the 2D blur is shift invariant, *i.e.*, if b[m, n; k, l] = b[m - k, n - l], then the superposition sum (1.4.17) becomes a convolution. In such cases, and for zero end conditions, the system matrix A has elements

$$a_{ij} = b[m(i) - m(j), n(i) - n(j)], \qquad (1.4.20)$$

and again has the block form (1.4.19) where the submatrices have elements

$$[\mathbf{A}_{nl}]_{mk} = b[m-k, n-l].$$
(1.4.21)

Because of the m - k dependence, each of the blocks in (1.4.19) is **Toeplitz** in this shift invariant case, so A is said to have **Toeplitz blocks**. Furthermore, because of the n - l dependence, all of the blocks along each "diagonal" in the block form (1.4.19) are the same, so A is said to be **block Toeplitz**. Combined, we say any such A is **block Toeplitz blocks** (**BTTB**) [54]. With a slight abuse of terminology, we will often simply call such matrices **Toeplitz**.

ASPIRE The command wt gen with system 0 generates a sparse A with this form.

MIRT The object Glsi_blur represents such system matrices as operators.

1.4.2.4 Separable 2D blur

If b[m, n; k, l] is a separable PSF, *i.e.*, if $b[m, n; k, l] = b_1[m; k] b_2[n; l]$, then the superposition sum (1.4.17) can be grouped as follows:

$$\bar{g}[m,n] = \sum_{l} b_2[n;l] \left(\sum_{k} b_1[m;k] f[k,l] \right).$$

The inner summation operates on the first index of f[m, n]; the outer summation operates on the second index. In this case the elements of A have the separable form

$$a_{ij} = b_1[m(i); m(j)] b_2[n(i); n(j)]$$

and the resulting matrix A has the special structure

$$\boldsymbol{A} = \boldsymbol{A}_2 \otimes \boldsymbol{A}_1, \tag{1.4.22}$$

where $A_1 \in \mathbb{R}^{M \times M}$ is one of the 1D matrix representations in §1.4 for the 1D PSF $b_1[m; k]$, $A_2 \in \mathbb{R}^{N \times N}$ is likewise defined in terms of $b_2[n; l]$, and " \otimes " denotes the Kronecker product defined in (28.1.12).

When A_1 and A_2 are each a Toeplitz matrix, such as when we use zero end conditions and a shift-invariant blur model, then $A_2 \otimes A_1$ is again block Toeplitz with Toeplitz blocks.

e,res,mat2,aij,si

e, res, mat2, Anlmk

For separable a separable PSF, there is another matrix representation that also can be useful. If G denotes the $M \times N$ matrix with elements g[m, n], and F denotes the matrix corresponding to f[m, n], then

$$\bar{\boldsymbol{G}} = \boldsymbol{A}_1 \boldsymbol{F} \boldsymbol{A}_2^T,$$

where A_1 and A_2 are the 1D blur matrices defined above. This expression is closely related to (1.4.22) because of the following property of vectorization:

$$\bar{\boldsymbol{y}} = \operatorname{vec}(\bar{\boldsymbol{G}}) = \operatorname{vec}(\boldsymbol{A}_1 \boldsymbol{F} \boldsymbol{A}_2^T) = (\boldsymbol{A}_2 \otimes \boldsymbol{A}_1) \operatorname{vec}(\boldsymbol{F}) = (\boldsymbol{A}_2 \otimes \boldsymbol{A}_1) \boldsymbol{x} = \boldsymbol{A} \boldsymbol{x}.$$
(1.4.23)

1.4.2.5 2D periodic end conditions

If we assume 2D periodic end conditions, *i.e.*, that $f[m, n] = f[m \mod M, n \mod N]$, also called **toroidal boundary** conditions, then the ordinary convolution (1.2.2) becomes a 2D circular convolution, defined by

$$\bar{g}[m,n] = \tilde{b}[m,n] \circledast_{M,N} f[m,n] \triangleq \sum_{k=0}^{M-1} \sum_{l=0}^{N-1} \tilde{b}[(m-k) \mod M, (n-l) \mod N] f[k,l],$$
(1.4.24)

where

$$\tilde{b}[m,n] \triangleq \sum_{k} \sum_{l} b[m-kM, n-lN]$$

Although periodic end conditions rarely (if ever) hold in practice, circulant models are convenient for analysis.

This circular convolution relationship has the matrix-vector representation $\bar{y} = Ax$ where the elements of the $MN \times MN$ matrix A are given by (cf. (1.4.20))

$$a_{ij} = b[(m(i) - m(j)) \mod M, (n(i) - n(j)) \mod N], \qquad i, j = 1, \dots, MN, \tag{1.4.25}$$

where $m(\cdot)$ and $n(\cdot)$ were defined in (1.4.15). Such a matrix is called **block circulant with circulant blocks** (**BCCB**). In particular, in this case A has the form (1.4.19) where

$$[\mathbf{A}_{nl}]_{mk} = \tilde{b}[(m-k) \mod M, (n-l) \mod N].$$

Example 1.4.1 See Fig. 1.4.3 for examples of the system matrix \mathbf{A} for a small image with M = 6 and N = 8. Each black rectangle outlines one of the (typically $N \times N$) blocks $\mathbf{A}_{nl} \in \mathbb{R}^{M \times M}$.

1.4.3 Circulant analysis of shift-invariant blur (s,res,circ)

For linear shift-invariant image restoration problems, A is always Toeplitz (or nearly Toeplitz depending on the chosen end conditions). However, most of the *methods* described in this *book* are also applicable to *shift-variant* problems, where the form of A depends on the physics and can be non-square and non-Toeplitz. For example, in tomography the elements of A correspond to a discretization of the **Radon transform**, which is usually non-square and hence non-Toeplitz. Despite the prevalence of non-Toeplitz problems, we can still obtain substantial insight by considering the Toeplitz case. In fact, we get the most signal processing *insight* by considering the case where A is circulant⁶, *i.e.*, the special family of Toeplitz matrices that correspond to periodic end conditions. Analysis using circulant matrices helps us relate matrix algebra solutions to signal processing principles. Equally importantly, circulant approximations are useful for reducing computation by replacing large matrix operations with simpler **fast Fourier transform** (**FFT**) calculations.

The link between circulant matrices and circular convolution is the **convolution property** of the **discrete Fourier transform** (**DFT**). We show next that "**circular convolution**" and "**circulant matrix**" are extremely closely related concepts.

⁶In analyses in later chapters, we will assume only that the square matrix A'A is circulant, rather than making such an assumption about the possibly non-square matrix A.



Figure 1.4.3: Illustration of system matrices A for 2D convolution for different end conditions, for M = 6 and N = 8. The upper-right figure illustrates (1.4.20), the lower-left figure illustrates (1.4.25), and the lower-right figure illustrates a 2D analogue of (1.4.9). Note that the spatial scale of the blur b[m, n] figure differs from the others.

s, res, circl 1.4.3.1 Circulant analysis in 1D (s, res, circ1)

In 1D, the convolution property of the discrete Fourier transform (DFT) can be expressed:

$$\bar{g}[n] = b[n] \circledast_N f[n] \stackrel{\text{DFT}}{\longleftrightarrow} \bar{G}_k = B_k F_k, \qquad (1.4.26)$$

where the N-point DFT of b[n] is the following:

$$b[n] \stackrel{\text{DFT}}{\longleftrightarrow} B_k \triangleq \sum_{n=0}^{N-1} b[n] e^{-i\frac{2\pi}{N}kn} = B(\Omega) \Big|_{\Omega = \frac{2\pi}{N}k}, \qquad k = 0, \dots, N-1, \qquad (1.4.27)$$

where the corresponding **discrete-time Fourier transform** (**DTFT**) of b[n] is

$$B(\Omega) \triangleq \sum_{n=-\infty}^{\infty} b[n] e^{-i\Omega n} .$$
(1.4.28)

Similarly F_k and \overline{G}_k are defined in terms of f[n] and $\overline{g}[n]$ respectively.

Mat | The convolution property (1.4.26) corresponds to the following MATLAB commands

g = ifft(fft(b) .* fft(f)), or equivalently, g = ifft(diag(fft(b)) * fft(f)).

It is useful to rewrite (1.4.26) in matrix-vector notation as

$$\underbrace{\begin{bmatrix} \bar{G}_0 \\ \vdots \\ \bar{G}_{N-1} \end{bmatrix}}_{N \times 1} = \underbrace{\begin{bmatrix} B_0 & \mathbf{0} \\ & \ddots \\ \mathbf{0} & B_{N-1} \end{bmatrix}}_{N \times N} \underbrace{\begin{bmatrix} F_0 \\ \vdots \\ F_{N-1} \end{bmatrix}}_{N \times 1} i.e., \ \vec{G} = \Gamma \vec{F},$$

where $\vec{G} = (\bar{G}_0, \dots, \bar{G}_{N-1})$ and $\vec{F} = (F_0, \dots, F_{N-1})$ are the vectors of N-point DFT coefficients of $\bar{g}[n]$ and f[n]respectively, and $\Gamma = \text{Diag}\{B_k\}$ is the $N \times N$ diagonal matrix with elements B_0, \ldots, B_{N-1} along its diagonal, where the B_k values were defined in (1.4.27). Defining the vector \bar{y} in terms of $\bar{g}[n]$ as in (1.4.5) and x in terms of f[n] as in (1.4.7), we have

$$\vec{G} = Q \, \bar{y}, \quad \vec{F} = Q x,$$

where Q is the $N \times N$ **DFT matrix** having elements

$$q_{nk} = e^{-i\frac{2\pi}{N}kn}, \qquad k, n = 0, \dots, N-1.$$
 (1.4.29)

The inverse 1D N-point DFT corresponds to the inverse of this matrix and is given by

$$Q^{-1} = \frac{1}{N}Q',$$
 (1.4.30)

where "Q'" denotes the Hermitian transpose of Q. Combining these relationships leads to a very useful tool for analysis, the following matrix-vector representation of the convolution property:

$$ar{y} = Q^{-1} \Gamma Q x.$$

Comparing the above relationships, we conclude that any circulant matrix, e.g., the system matrix (1.4.13), has the following matrix decomposition:

$$\boldsymbol{A} = \boldsymbol{Q}^{-1} \boldsymbol{\Gamma} \boldsymbol{Q} = \frac{1}{N} \boldsymbol{Q}' \boldsymbol{\Gamma} \boldsymbol{Q}. \tag{1.4.31}$$

This is an eigenvector decomposition with eigenvalues $\{B_k\}$. So the eigenvalues of any circulant matrix are the DFT coefficients of the first column of that matrix. When viewing an expression like (1.4.31), one can think of A as a (circularly shift-invariant) filter whose frequency response is embedded in the diagonal elements of Γ .

Mat Although Q is used primarily for theoretical analysis, if needed it can be computed in MATLAB for modest values of N using Q = dftmtx(N).

s, res, circ2 1.4.3.2 Circulant analysis in 2D (s, res, circ2)

The frequency-domain expression corresponding to 2D circular convolution (1.4.24) is

$$\bar{G}[k,l] = B[k,l] F[k,l], \qquad k = 0, \dots, M-1, \ l = 0, \dots, N-1,$$

where the $(M \times N)$ -point **2D DFT** of $\tilde{b}[m, n]$ is defined as follows:

$$B[k,l] = \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} e^{-i(2\pi m k/M + 2\pi n l/N)} \tilde{b}[m,n]$$

=
$$\sum_{n=0}^{N-1} e^{-i2\pi n l/N} \left[\sum_{m=0}^{M-1} e^{-i2\pi m k/M} \tilde{b}[m,n] \right].$$
(1.4.32)

If we order lexicographically the 2D DFT coefficients $\{F[k, l]\}$ as a MN vector F and the 2D image f[m, n] as a MN vector x per (1.4.14), then we can express the 2D DFT by a linear operator, *i.e.*, F = Qx, where Q denotes the following $MN \times MN$ matrix

$$\boldsymbol{Q} = \boldsymbol{Q}_N \otimes \boldsymbol{Q}_M, \tag{1.4.33}$$

where Q_N denotes the 1D N-point DFT matrix defined in (1.4.29). One can also derive (1.4.33) using the vectorization property in (1.4.23). The double sum in the 2D DFT expression (1.4.32) becomes the above **Kronecker product** when expressed in matrix notation. (See §28.1.6.) Thus, a circulant-block-circulant system matrix defined by (1.4.25) has the following eigenvector decomposition:

$$\boldsymbol{A} = \boldsymbol{Q}^{-1} \boldsymbol{\Gamma} \boldsymbol{Q} = \frac{1}{MN} \boldsymbol{Q}' \boldsymbol{\Gamma} \boldsymbol{Q},$$

where Γ is a diagonal matrix with diagonal elements that are the eigenvalues of A, namely the 2D DFT coefficients $\{B[k, l]\}$ ordered lexicographically. So in 2D (and higher) we get the same form as (1.4.31) but with Q corresponding to a DFT of whatever dimension we are using. This decomposition is central to subsequent analyses.

Caution! In 1D the eigenvalues of a circulant matrix A were simply the 1D DFT coefficients of its first column. To find such eigenvalues in 2D, we take the first column of A and reshape it into a $M \times N$ array, and then compute the 2D DFT of that array.

1.5 Simple restoration methods (s,res,inv)

Having established two convenient notations, we return to the image restoration problem of recovering f[m, n] from g[m, n] under the model (1.2.3). We describe two "solutions," both of which are inadequate in general, for essentially the same reason, as will be analyzed.

1.5.1 The deconvolution solution

The convolution property of the Fourier transform (1.4.1), where $\bar{G}(\Omega_1, \Omega_2) = B(\Omega_1, \Omega_2) F(\Omega_1, \Omega_2)$, suggests the following inverse-filter solution:

$$\hat{F}(\Omega_1, \Omega_2) = \begin{cases} G(\Omega_1, \Omega_2) / B(\Omega_1, \Omega_2), & B(\Omega_1, \Omega_2) \neq 0 \\ ?, & B(\Omega_1, \Omega_2) = 0. \end{cases}$$
(1.5.1)

Equivalently,

$$f[m,n] = b_{\rm inv}[m,n] ** g[m,n]$$

where $b_{inv}[m, n]$ is the inverse Fourier transform of $1/B(\Omega_1, \Omega_2)$. Such restoration methods are called **deconvolu**tion. Unfortunately, usually b[m, n] is a lowpass type of filter, so $B(\Omega_1, \Omega_2)$ is zero or near zero for high spatial frequencies. So the simple inverse filter approach greatly amplifies high spatial-frequency noise. This property should be unsurprising because we did not consider noise when proposing (1.5.1).

Similar noise-amplifying phenomena are present in typical analytical solutions to tomographic reconstruction problems, because those solutions also ignore noise in the problem formulation. This book emphasizes methods where noise considerations are fundamental to the formulation.

[RQ2]

e.dft2

1.5.2 The matrix inverse solution

By examining the matrix-vector expression (1.4.4), one could be tempted to propose the solution

$$\hat{\boldsymbol{x}} = \boldsymbol{A}^{-1}\boldsymbol{y},\tag{1.5.2}$$

at least when A is an invertible (and hence square) matrix [69]. We analyze this type of solution in more detail in Chapter 17, where the desirability of **regularization** is emphasized. For initial understanding of why this matrix inverse solution is inadequate, consider the case where A is circulant (*e.g.*, (1.4.13)) so that the decomposition (1.4.31) applies. Then we have $A^{-1} = Q^{-1} \Gamma^{-1} Q$ so

$$\hat{\boldsymbol{x}} = \boldsymbol{Q}^{-1} \boldsymbol{\Gamma}^{-1} \boldsymbol{Q} \boldsymbol{y}.$$

This solution is essentially the same as (1.5.1) because Q corresponds to the DFT and Γ^{-1} has reciprocals of samples of the system frequency response $B(\Omega_1, \Omega_2)$ along its diagonal. Solutions of the form (1.5.2) are known as algebraic reconstruction techniques because they are based on linear algebra concepts only. Hereafter we will focus on methods that use linear algebra combined with appropriate statistical considerations. [RQ3]

e,res,x=A,inv,v

Statistical image restoration (s,res,stat)

s.res.stat

1.6

Statistical methods for image restoration improve on the simple methods described in \$1.5 by incorporating both statistical models for the noise in the measurements y and prior knowledge about the unknown object x.

If one has confidence in the statistical model for y (and perhaps in a statistical model for x as well), then a theoretically appealing approach is to apply the tools of estimation theory to find an estimator $\hat{x} = \hat{x}(y)$ of x.

Even within the framework of statistical estimation one must choose between differing philosophical approaches. The most frequently studied methods are **maximum-likelihood** (ML) estimation, **Bayesian estimation**, and **regularized**- or **penalized-likelihood** estimation, all of which are described next. These approaches apply both to image restoration and to image reconstruction.

s, res, noise 1.6.1 Noise models (s, res, noise)

This section summarizes a few of the statistical models for the measurement noise that are most popular in image restoration problems. Once again, the matrix-vector notation facilitates the presentation.

1.6.1.1 Additive gaussian noise

The most prevalent statistical model for image restoration problems corresponds to (1.2.3), *i.e.*,

$$\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{\varepsilon}, \tag{1.6.1}$$

where $y, \varepsilon \in \mathbb{R}^{n_{d}}, x \in \mathbb{R}^{n_{p}}$, and $A \in \mathbb{R}^{n_{d} \times n_{p}}$. For a $M \times N$ image, for most cases, including where zero end conditions are used, we have $n_{p} = n_{d} = MN$. But we may have $n_{d} \neq n_{p}$ for other end conditions, such as the extended end conditions, and for other image recovery problems.

To describe the noise statistics, we will often refer to the $n_d \times n_d$ covariance matrix of ε , defined by

$$K_{\varepsilon} = \operatorname{Cov}\{\varepsilon\} = \mathsf{E}[(\varepsilon - \mathsf{E}[\varepsilon])(\varepsilon - \mathsf{E}[\varepsilon])'], \qquad (1.6.2)$$

where $E[\cdot]$ denotes statistical expectation. The elements of K_{ε} are given as follows:

$$[\mathbf{K}_{\boldsymbol{\varepsilon}}]_{ij} = \mathbf{e}'_i \mathbf{K}_{\boldsymbol{\varepsilon}} \mathbf{e}_j = \mathsf{Cov}\{\varepsilon_i, \varepsilon_j\} = \mathsf{E}[(\varepsilon_i - \mathsf{E}[\varepsilon_i])(\varepsilon_j - \mathsf{E}[\varepsilon_j])],$$
(1.6.3)

where e_j denotes the *j*th **unit vector** of length n_d .

Usually one assumes that additive noise has a gaussian distribution with zero mean and a known covariance matrix K_{ε} that is symmetric positive definite. Then (1.6.1) is equivalent to saying that y is a gaussian random vector with the following probability density function (pdf):

$$\mathsf{p}(\boldsymbol{y} \mid \boldsymbol{x}) = \frac{1}{\sqrt{(2\pi)^{n_{\mathrm{d}}} \det\{\boldsymbol{K}_{\boldsymbol{\varepsilon}}\}}} \exp\left(-\frac{1}{2}(\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x})'\boldsymbol{K}_{\boldsymbol{\varepsilon}}^{-1}(\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x})\right), \tag{1.6.4}$$

where det{ K_{ε} } denotes the **determinant** of the noise **covariance matrix** K_{ε} .

1.6.1.2 Poisson measurements

For some illumination conditions, the random quantum effects of photons may dominate over other sources of measurement errors. This variability is called **shot noise**. Often the statistics of these effects are modeled by Poisson distributions, so an alternative to (1.6.1) is to assume that the elements y_i of the measurement vector y are independent Poisson random variables whose means are given by the *i*th element of Ax. To denote such independent Poisson variates, we write

$$y_i \sim \mathsf{Poisson}\{\bar{y}_i(\boldsymbol{x})\}, \quad i = 1, \dots, n_{\mathrm{d}},$$

$$(1.6.5)$$

where $y_i \in \{0, 1, 2, ...\}$ and where

$$\bar{y}_i(\boldsymbol{x}) \triangleq \mathsf{E}[y_i \,|\, \boldsymbol{x}] = [\boldsymbol{A}\boldsymbol{x}]_i = \sum_{j=1}^{n_{\mathrm{p}}} a_{ij} x_j.$$

e,res,y=A*x+e

⁷The notation " $\boldsymbol{x} \in \mathbb{R}^{n_{\mathrm{P}}}$ " indicates that \boldsymbol{x} is a column vector of length n_{P} .

$$\mathsf{P}\{\boldsymbol{y} \,|\, \boldsymbol{x}\} = \prod_{i=1}^{n_{\rm d}} \mathsf{P}\{y_i \,|\, \boldsymbol{x}\} = \prod_{i=1}^{n_{\rm d}} \mathrm{e}^{-[\boldsymbol{A}\boldsymbol{x}]_i} \,([\boldsymbol{A}\boldsymbol{x}]_i)^{y_i} / (y_i!), \tag{1.6.6}$$

where "!" denotes the factorial. This model is particularly appropriate for measurement systems that count photon interactions, as described in Chapter 8.

1.6.1.3 Poisson+gaussian measurements

The additive gaussian noise model of (1.6.1) is inexact in optical imaging systems such as those using **CCD arrays** [7, 8]. A more realistic model would account for the quantum effects of photons that interact with the detector, as well as the additional noise in the readout electronics. A combination of Poisson and gaussian distributions is appropriate for such systems, although the resulting distribution is somewhat inconvenient and requires approximation for practical implementation [7, 8].

Similar inconveniences arise in PET scans that are precorrected for random coincidences [70, 71], and in X-ray CT systems with current integrating detectors [72].

1.6.2 Maximum-likelihood estimation (s,res,stat,ml)

One can think of a statistical model p(y | x) as quantifying the "agreement" between the measurement vector y and a candidate object vector x. For maximum-likelihood estimation, one finds the x that maximizes this agreement, *i.e.*, the \hat{x} that best fits the data, using the log-likelihood

$$L(\boldsymbol{x}) \triangleq \log p(\boldsymbol{y} \mid \boldsymbol{x}).$$

(Typically the dependence of L on the data y is suppressed in the notation because we have only one vector y in a given experiment, but need to consider many candidate x vectors.) The ML estimator is defined by

$$\hat{\boldsymbol{x}}_{\scriptscriptstyle\mathrm{ML}} = rg\max_{\boldsymbol{x}} \mathsf{L}(\boldsymbol{x}),$$

where the maximization is restricted to the set of acceptable values of x. For example, often we only allow vectors x having nonnegative elements because light intensity is nonnegative.

1.6.2.1 Poisson noise and the Richardson-Lucy iteration

The log-likelihood associated with the Poisson model (1.6.6) is

$$\mathsf{L}(\boldsymbol{x}) \equiv \sum_{i=1}^{n_{\mathrm{d}}} y_i \log([\boldsymbol{A}\boldsymbol{x}]_i) - [\boldsymbol{A}\boldsymbol{x}]_i = \boldsymbol{y}' \log(\boldsymbol{A}\boldsymbol{x}) - \mathbf{1}' \boldsymbol{A}\boldsymbol{x},$$

where we use the nonstandard (but convenient) notation " \equiv " to indicate that the two expressions differ only by an **irrelevant constant** that is independent of x, and here log acts element-wise on a vector argument. Lucy considered this model [73], and derived the following iteration⁸:

$$x_j^{(n+1)} = \frac{x_j^{(n)}}{\sum_{i=1}^{n_{\rm d}} a_{ij}} \sum_{i=1}^{n_{\rm d}} a_{ij} y_i / [\boldsymbol{A}\boldsymbol{x}^{(n)}]_i.$$
(1.6.7)

Richardson had earlier derived this same iteration using Bayes rule [74]. In the image restoration field, this is known as the **Richardson-Lucy** (or **Lucy-Richardson**) deconvolution procedure. It turns out to be the same formula as the ML-EM algorithm for emission tomography, as described in detail in Chapter 18. An appealing characteristic of the iteration (1.6.7) is that if the initial image $x^{(0)}$ is nonnegative, then so are all the iterates $\{x^{(n)}\}$. However, as the iterations proceed the images become increasingly noisy, due to the nature of unregularized ML restoration.

MIRT See eml_em.m.

⁸Lucy's derivation assumed $\sum_{i=1}^{n_{d}} a_{ij} = 1$.

1.6.2.2 Gaussian noise

The limitations of the ML approach are illustrated easily by considering the gaussian model (1.6.4), for which the log-likelihood is

$$\begin{split} \mathsf{L}(\boldsymbol{x}) &= -\frac{1}{2}(\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x})'\boldsymbol{K}_{\varepsilon}^{-1}(\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}) - \frac{1}{2}\log(\det\{2\pi\boldsymbol{K}_{\varepsilon}\})\\ &\equiv -\frac{1}{2}(\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x})'\boldsymbol{K}_{\varepsilon}^{-1}(\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}) = -\frac{1}{2}\left\|\boldsymbol{K}_{\varepsilon}^{-1/2}\left(\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}\right)\right\|_{2}^{2}. \end{split}$$

This L(x) is a concave function (see §29.9). If A has full column rank (which is rare in deblurring problems due to zeros in the frequency response), then the ML estimate for gaussian noise is

$$\hat{\boldsymbol{x}}_{\text{ML}} = \left[\boldsymbol{A}'\boldsymbol{K}_{\varepsilon}^{-1}\boldsymbol{A}\right]^{-1}\boldsymbol{A}'\boldsymbol{K}_{\varepsilon}^{-1}\boldsymbol{y}.$$
(1.6.8)

In addition to having full column rank, if A is also square then it is **invertible**, and the unconstrained maximizer of L is

$$\hat{\boldsymbol{x}}_{\mathrm{ML}} = \boldsymbol{A}^{-1}\boldsymbol{y}. \tag{1.6.9}$$

So the ML estimation criterion can again lead to the "inverse" solution (1.5.2), yielding unacceptably noisy images in most practical problems.

To reduce this noise, one must impose some type of **constraints** on the estimator \hat{x} , or otherwise incorporate prior information about x. Bayesian estimation and penalized-likelihood estimation are two related ways to achieve this goal.

1.7 Bayesian estimation (s,res,stat,bayes)

For ML estimation, the only statistical model required is that of the measurements, namely the likelihood p(y | x). For **Bayesian estimation**, one must also postulate a probability distribution p(x) for the unknown object vectors. This distribution is called the **prior distribution** for x, because it describes object properties that are assumed to be "known" *before* the measurements y are acquired.

1.7.1 MMSE estimation

Given a statistical model p(y | x) and a prior p(x), in the Bayesian framework one can devise estimators that minimize an expected cost, called the **risk** or **loss**, averaged over the family of possible objects x. The simplest risk function is simply the **mean-squared error** (MSE) of an estimator \hat{x} , defined by

$$MSE(\hat{\boldsymbol{x}}) = \mathsf{E}\Big[\|\hat{\boldsymbol{x}} - \boldsymbol{x}\|^2\Big] = \iint \|\hat{\boldsymbol{x}}(\boldsymbol{y}) - \boldsymbol{x}\|^2 \,\mathsf{p}(\boldsymbol{y} \,|\, \boldsymbol{x}) \,\mathsf{p}(\boldsymbol{x}) \,\mathrm{d}\boldsymbol{y} \,\mathrm{d}\boldsymbol{x} \,.$$

A classical result in Bayesian estimation theory [75, p. 419] is that the minimum mean-squared error (MMSE) estimator for x given y is the following conditional expectation or conditional mean:

$$\hat{\boldsymbol{x}}_{\text{MMSE}} = \underset{\hat{\boldsymbol{x}}}{\operatorname{arg\,min\,MSE}} (\hat{\boldsymbol{x}}) = \mathsf{E}[\boldsymbol{x} \,|\, \boldsymbol{y}] = \int \boldsymbol{x} \, \mathsf{p}(\boldsymbol{x} \,|\, \boldsymbol{y}) \, \mathrm{d}\boldsymbol{x} \,. \tag{1.7.1}$$

Unfortunately this conditional expectation is difficult to compute for many problems, so MMSE estimation is used only in relatively rare cases.

In general the MMSE estimator is nonlinear. If this is undesirable or intractable, another option is to try to find the *linear* or *affine* estimator that minimizes MMSE. This too can be challenging in cases where the MSE is itself analytically intractable.

1.7.2 MAP estimation

In part because of these difficulties, the Bayesian estimator that is often used in practice is the maximum *a posteriori* (MAP) approach, defined as the maximizer of the posterior distribution p(x | y) as follows:

$$\hat{\boldsymbol{x}}_{\text{map}} = rg\max_{\boldsymbol{x}} \mathsf{p}(\boldsymbol{x} \,|\, \boldsymbol{y}) \,.$$

e, res, xh, ml, inv

[RQ4]

e,res,mmse

This approach finds the image that has the highest posterior probability⁹ given the data y. By Bayes' rule:

$$\mathsf{p}(\boldsymbol{x} \,|\, \boldsymbol{y}) = rac{\mathsf{p}(\boldsymbol{y} \,|\, \boldsymbol{x}) \,\mathsf{p}(\boldsymbol{x})}{\mathsf{p}(\boldsymbol{y})},$$

where, by total probability, the overall data distribution $p(y) = \int p(y | \tilde{x}) p(\tilde{x}) d\tilde{x}$ is independent of the true, unknown value of the image x. Because the logarithm function is monotone, an equivalent formulation is:

$$\hat{\boldsymbol{x}}_{\text{MAP}} = \arg\max_{\boldsymbol{x}} \left[\log \mathsf{p}(\boldsymbol{y} \,|\, \boldsymbol{x}) + \log \mathsf{p}(\boldsymbol{x}) \right], \tag{1.7.2}$$

where we can ignore $\log p(y)$ because it is independent of x.

In a few special cases there are analytical expressions for the MAP estimator. However, most interesting problems lack such an analytical solution, so an iterative algorithm is needed to perform the maximization. Such iterative algorithms are a primary focus of this *book*.

A philosophical difficulty with the Bayesian paradigm is that the "priors" p(x) that are commonly used in Bayesian image restoration methods capture only very local properties of images. If one generates random draws from typical Bayesian image priors, the results look very little like natural images. (See Fig. 1.7.1.) This is contrary to the usual sense of the term "prior" in statistical estimation, where values drawn from the prior distribution are representative of the objects under investigation.

stat, gauss 1.7.3 Bayesian estimation in linear gaussian models (s,res,stat,gauss)

As a concrete example of Bayesian estimation, we consider the linear model (1.6.1) with additive gaussian noise and assume that the prior distribution for x is also gaussian. This example is one of the few where analytical solutions are available. The MAP and MMSE estimators turn out to be identical in this problem, unlike in more general cases.

Specifically, consider the following statistical assumptions.

- $oldsymbol{y} = oldsymbol{A} oldsymbol{x} + oldsymbol{arepsilon}$ with $oldsymbol{A} \in \mathbb{R}^{n_{ ext{d}} imes n_{ ext{p}}}$
- $\varepsilon \sim \mathsf{N}(\mathbf{0}, K_{\varepsilon})$
- $\boldsymbol{x} \sim \mathsf{N}(\boldsymbol{\mu}_{\boldsymbol{x}}, \boldsymbol{K}_{\boldsymbol{x}})$
- ε and x are independent
- μ_x , K_{ε} , and K_x are all known.

Due to the independence of x and ε , the likelihood is:

p

$$(\boldsymbol{y} \mid \boldsymbol{x}) = p_{\boldsymbol{y} \mid \boldsymbol{x}} (\boldsymbol{A} \boldsymbol{x} + \boldsymbol{\varepsilon} \mid \boldsymbol{x}) = p_{\boldsymbol{\varepsilon}} (\boldsymbol{y} - \boldsymbol{A} \boldsymbol{x})$$
$$= \frac{1}{\sqrt{(2\pi)^{n_{d}} \det\{\boldsymbol{K}_{\boldsymbol{\varepsilon}}\}}} e^{-\frac{1}{2}(\boldsymbol{y} - \boldsymbol{A} \boldsymbol{x})' \boldsymbol{K}_{\boldsymbol{\varepsilon}}^{-1}(\boldsymbol{y} - \boldsymbol{A} \boldsymbol{x})}.$$
(1.7.3)

By assumption, the prior distribution for x is:

$$\mathsf{p}(\boldsymbol{x}) = \frac{1}{\sqrt{(2\pi)^{n_{\mathrm{p}}} \det\{\boldsymbol{K}_{\boldsymbol{x}}\}}} e^{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_{\boldsymbol{x}})'\boldsymbol{K}_{\boldsymbol{x}}^{-1}(\boldsymbol{x}-\boldsymbol{\mu}_{\boldsymbol{x}})}.$$
 (1.7.4)

s, res, map, gauss 1.7.3.1 MAP estimator

Combining the likelihood and the prior leads to the following form for the MAP estimator:

$$egin{aligned} \hat{m{x}}_{\scriptscriptstyle\mathrm{MAP}} &= rg\max_{m{x}} \left[\log \mathsf{p}(m{y} \,|\, m{x}) + \log \mathsf{p}(m{x})
ight] \ &= rg\min_{m{x}} \Psi(m{x}), \end{aligned}$$

where we ignore irrelevant constants in defining the following cost function (also known as a loss function):

$$\Psi(\boldsymbol{x}) \triangleq \frac{1}{2}(\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x})'\boldsymbol{K}_{\varepsilon}^{-1}(\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}) + \frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu}_{\boldsymbol{x}})'\boldsymbol{K}_{\boldsymbol{x}}^{-1}(\boldsymbol{x} - \boldsymbol{\mu}_{\boldsymbol{x}}).$$
(1.7.5)

⁹The MAP estimator also minimizes the "hit-or-miss" risk function [76, p. 343]. The suitability of that risk function for imaging problems is somewhat debatable because it assigns the same loss to *all* incorrect estimates. For a discussion of a canonical loss function, see [77].

This cost function consists of a **data-fit** or **discrepancy** term and a **prior** term. By expanding $\Psi(x)$ and **completing the square**, one can show that

$$\Psi(\boldsymbol{x}) \equiv \frac{1}{2} \left\| \boldsymbol{H}^{1/2} \boldsymbol{x} - \boldsymbol{H}^{-1/2} (\boldsymbol{A}' \boldsymbol{K}_{\varepsilon}^{-1} \boldsymbol{y} + \boldsymbol{K}_{\boldsymbol{x}}^{-1} \boldsymbol{\mu}_{\boldsymbol{x}}) \right\|^{2},$$

where ${}^{10} H \triangleq A' K_{\varepsilon}^{-1} A + K_{x}^{-1}$. It is clear from the preceding expression that a minimizer of $\Psi(x)$ is

$$\begin{aligned} \hat{x}_{\text{MAP}} &= \boldsymbol{H}^{-1} (\boldsymbol{A}' \boldsymbol{K}_{\varepsilon}^{-1} \boldsymbol{y} + \boldsymbol{K}_{\boldsymbol{x}}^{-1} \boldsymbol{\mu}_{\boldsymbol{x}}) \\ &= \left[\boldsymbol{A}' \boldsymbol{K}_{\varepsilon}^{-1} \boldsymbol{A} + \boldsymbol{K}_{\boldsymbol{x}}^{-1} \right]^{-1} (\boldsymbol{A}' \boldsymbol{K}_{\varepsilon}^{-1} \boldsymbol{y} + \boldsymbol{K}_{\boldsymbol{x}}^{-1} \boldsymbol{\mu}_{\boldsymbol{x}}) \\ &= \boldsymbol{\mu}_{\boldsymbol{x}} + \left[\boldsymbol{A}' \boldsymbol{K}_{\varepsilon}^{-1} \boldsymbol{A} + \boldsymbol{K}_{\boldsymbol{x}}^{-1} \right]^{-1} \boldsymbol{A}' \boldsymbol{K}_{\varepsilon}^{-1} (\boldsymbol{y} - \boldsymbol{A} \boldsymbol{\mu}_{\boldsymbol{x}}). \end{aligned}$$
(1.7.6)

Finding the minimizer of a function by "completing the square" is rarely a convenient approach. An alternative is to equate the gradient of $\Psi(x)$ to zero, provided no constraints such as nonnegativity are desired. Let ∇f denote the **row gradient** of a function $f : \mathbb{R}^{n_p} \to \mathbb{R}$, *i.e.*,

$$abla f(\boldsymbol{x}) = \left[rac{\partial}{\partial x_1} f(\boldsymbol{x}) \ \dots \ rac{\partial}{\partial x_{n_{\mathrm{P}}}} f(\boldsymbol{x})
ight].$$

Then one can easily verify the following very useful gradient relationships

- $abla_{m{x}} m{v}' m{x} = m{v}'$ for $m{v} \in \mathbb{R}^{n_{\mathrm{p}}}$
- $abla x rac{1}{2} x' M x = x' rac{1}{2} (M+M') ext{ for } M \in \mathbb{R}^{n_{ ext{p}} imes n_{ ext{p}}}$.

We let ∇ denote the **column gradient** operator, the transpose of ∇ . It follows that

$$\begin{aligned} \nabla_{\boldsymbol{x}} \frac{1}{2} (\boldsymbol{y} - \boldsymbol{A} \boldsymbol{x})' \boldsymbol{K}_{\varepsilon}^{-1} (\boldsymbol{y} - \boldsymbol{A} \boldsymbol{x}) \\ &= \nabla_{\boldsymbol{x}} \left[\frac{1}{2} \boldsymbol{y}' \boldsymbol{K}_{\varepsilon}^{-1} \boldsymbol{y} - \boldsymbol{y}' \boldsymbol{K}_{\varepsilon}^{-1} \boldsymbol{A} \boldsymbol{x} + \frac{1}{2} \boldsymbol{x}' \boldsymbol{A}' \boldsymbol{K}_{\varepsilon}^{-1} \boldsymbol{A} \boldsymbol{x} \right] \\ &= -\boldsymbol{A}' \boldsymbol{K}_{\varepsilon}^{-1} \boldsymbol{y} + \boldsymbol{A}' \boldsymbol{K}_{\varepsilon}^{-1} \boldsymbol{A} \boldsymbol{x} \\ &= -\boldsymbol{A}' \boldsymbol{K}_{\varepsilon}^{-1} (\boldsymbol{y} - \boldsymbol{A} \boldsymbol{x}). \end{aligned}$$

Using these properties, the column gradient of $\Psi(x)$ defined in (1.7.5) above is

$$egin{aligned} &
abla \Psi(oldsymbol{x}) = -oldsymbol{A}'oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}(oldsymbol{y} - oldsymbol{A}oldsymbol{x}) + oldsymbol{K}_{oldsymbol{x}}^{-1}(oldsymbol{x} - oldsymbol{\mu}_{oldsymbol{x}}) + [oldsymbol{A}'oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}(oldsymbol{x} - oldsymbol{A}) + [oldsymbol{A}'oldsymbol{K}_{oldsymbol{x}}^{-1}(oldsymbol{x} - oldsymbol{\mu}_{oldsymbol{x}}) + [oldsymbol{A}'oldsymbol{K}_{oldsymbol{x}}^{-1}(oldsymbol{x} - oldsymbol{\mu}_{oldsymbol{x}}) + [oldsymbol{A}'oldsymbol{K}_{oldsymbol{x}}^{-1}(oldsymbol{x} - oldsymbol{\mu}_{oldsymbol{x}}) + [oldsymbol{A}'oldsymbol{K}_{oldsymbol{x}}^{-1}(oldsymbol{x} - oldsymbol{X}_{oldsymbol{x}}) + [oldsymbol{A}'oldsymbol{K}_{oldsymbol{x}}^{-1}(oldsymbol{x} - oldsymbol{X}_{oldsymbol{x}}) + [oldsymbol{A}'oldsymbol{K}_{oldsymbol{x}}^{-1}(oldsymbol{x} - oldsymbol{X}_{oldsymbol{x}}) + [oldsymbol{A}'oldsymbol{K}_{oldsymbol{x}}^{-1}(oldsymbol{x} - oldsymbol{X}_{oldsymbol{x}}) + [oldsymbol{A}'oldsymbol{K}_{oldsymbol{x}}^{-1}(oldsymbol{X}_{oldsymbol{x}}) + [oldsymbol{A}'oldsymbol{X}_{oldsymbol{x}}^{-1}(oldsymbol{x} - oldsymbol{X}_{$$

Equating this gradient to zero yields the MAP estimator

$$\hat{x}_{\text{MAP}} = \mu_{x} + \left[A'K_{\varepsilon}^{-1}A + K_{x}^{-1}\right]^{-1}A'K_{\varepsilon}^{-1}(y - A\mu_{x}),$$

which is equivalent to (1.7.6).

What happens to the MAP estimator as our confidence in the prior information decreases? If $K_x \to \infty$, then $K_x^{-1} \to 0$ and

$$\hat{oldsymbol{x}}_{\scriptscriptstyle{\mathrm{MAP}}}
ightarrow \left[oldsymbol{A}'oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}oldsymbol{A}'oldsymbol{arepsilon}^{-1}oldsymbol{A}'oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}oldsymbol{A}'oldsymbol{arepsilon}^{-1}oldsymbol{A}'oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}oldsymbol{A}'oldsymbol{arepsilon}^{-1}oldsymbol{A}'oldsymbol{A}'oldsymbol{arepsilon}}^{-1}oldsymbol{A}'oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}oldsymbol{A}'oldsymbol{arepsilon}^{-1}oldsymbol{A}'oldsym$$

which is the conventional weighted least-squares (WLS) estimator, which also happens to be the ML estimator in this case. In particular, if $K_{\varepsilon} = \sigma^2 I$ and A is invertible, then $\hat{x}_{MAP} \to A^{-1}y$, the inverse estimator. So the prior information is essential to avoid the noise problems associated with ML estimation.

A significant practical problem with this analytical solution is the apparent need to "invert" large matrices. In practice we usually minimize $\Psi(x)$ with an iterative algorithm, *e.g.*, Chapter 16, rather than using the explicit analytical form.

¹⁰The matrix **H** is invertible because $A' K_{\varepsilon}^{-1} A$ is positive semidefinite and K_x^{-1} is positive definite so their sum is positive definite.

1.7.3.2 MMSE estimator

Because x and y are jointly gaussian under the assumptions in this example, it is straightforward to evaluate the conditional mean estimator (1.7.1). In general for jointly gaussian random vectors [78, p. 302] [76, p. 325], the conditional mean has the following form:

$$\mathsf{E}[\boldsymbol{x} \,|\, \boldsymbol{y}] = \mathsf{E}[\boldsymbol{x}] + \mathsf{Cov}\{\boldsymbol{x}, \boldsymbol{y}\} \,\mathsf{Cov}\{\boldsymbol{y}\}^{-1}(\boldsymbol{y} - \mathsf{E}[\boldsymbol{y}]).$$

In this case, $Cov\{x, y\} = Cov\{x, Ax + \varepsilon\} = K_x A'$ and $Cov\{y\} = Cov\{Ax + \varepsilon\} = AK_x A' + K_{\varepsilon}$, so the MMSE estimator has the following affine form:

$$\hat{\boldsymbol{x}}_{\text{MMSE}} = \boldsymbol{\mu}_{\boldsymbol{x}} + \boldsymbol{K}_{\boldsymbol{x}} \boldsymbol{A}' \left[\boldsymbol{A} \boldsymbol{K}_{\boldsymbol{x}} \boldsymbol{A}' + \boldsymbol{K}_{\boldsymbol{\varepsilon}} \right]^{-1} (\boldsymbol{y} - \boldsymbol{A} \boldsymbol{\mu}_{\boldsymbol{x}}).$$
(1.7.8)

Using the **matrix inversion lemma** (see (28.1.9) and (28.1.10)), one can show that this expression is identical to (1.7.6). Thus, the MAP and MMSE estimators are identical in this linear gaussian problem. This gives further motivation for using MAP estimation because many problems are "nearly" gaussian.

1.7.3.3 Interpretation of MAP/MMSE estimators

For the linear gaussian model with a gaussian prior, we can rewrite the MAP/MMSE estimators in (1.7.6) and (1.7.8) as follows:

$$\hat{oldsymbol{x}}_{ ext{MAP/MMSE}} = ig[oldsymbol{A}'oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}oldsymbol{A}+oldsymbol{K}_{oldsymbol{x}}^{-1}oldsymbol{y} + ig(oldsymbol{I} - ig[oldsymbol{A}'oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}oldsymbol{A}+oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}oldsymbol{A}'oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}oldsymbol{y} + ig(oldsymbol{I} - ig[oldsymbol{A}'oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}oldsymbol{A}+oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}oldsymbol{A}'oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}oldsymbol{y} + ig(oldsymbol{I} - ig[oldsymbol{A}'oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}oldsymbol{A}+oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}oldsymbol{A}'oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}oldsymbol{y} + ig(oldsymbol{I} - ig[oldsymbol{A}'oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}oldsymbol{A}+oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}oldsymbol{A}'oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}oldsymbol{y} + ig(oldsymbol{A}+oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}oldsymbol{A}+oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}oldsymbol{A}+oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}oldsymbol{A}+oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}oldsymbol{Y}+oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}oldsymbol{A}+oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}oldsymbol{A}+oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}oldsymbol{A}+oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}oldsymbol{A}+oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}oldsymbol{A}+oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}oldsymbol{A}+oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}oldsymbol{A}+oldsymbol{K}_{oldsymbol{arepsilon}}^{-1}oldsymbol{A}+oldsymbol{A}+oldsymbol{ella}+oldsymbol{A}+oldsymbol{$$

The first term depends on the data, whereas the second term depends on the prior mean image μ_x . In other words, the second term is unrelated to the measurements, so it could be viewed before taking any data! That term would be important quantitatively in terms of minimizing MSE, but qualitatively it provides no useful "new" information. All of the useful information about the scene (or patient in the medical context) is in the first term that depends on the data y. Therefore in my view it is best to simply choose $\mu_x = 0$ (or adopt another approach altogether) in which case the second term disappears. Indeed most modern image reconstruction methods do not include any μ_x term. The first term above also depends on the prior covariance K_x , and that prior can strongly influence the image quality as shown below.

1.7.3.4 White gaussian case

The simplest special case of this MAP estimator is when the noise is white and gaussian, *i.e.*, $K_{\varepsilon} = \sigma^2 I$, and when one assumes that the object vector is zero mean ($\mu_x = 0$) and has independent and identically distributed components, *i.e.*, $K_x = \frac{1}{\beta}I$. Under these (unrealistic) assumptions, the cost function is a simple combination of a least-squares data-fit term (negative log-likelihood) and an energy penalty term:

$$\Psi(\boldsymbol{x}) = \frac{1}{2\sigma^2} \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}\|^2 + \frac{1}{2}\beta \|\boldsymbol{x}\|^2$$
(1.7.9)

and the corresponding MAP estimator simplifies to:

$$\hat{\boldsymbol{x}}_{\text{MAP}} = \operatorname*{arg\,min}_{\boldsymbol{x}} \Psi(\boldsymbol{x}) = \left[\boldsymbol{A}'\boldsymbol{A} + \beta\sigma^2 \boldsymbol{I}\right]^{-1} \boldsymbol{A}'\boldsymbol{y}. \tag{1.7.10}$$

In statistics, this estimation method is known as ridge regression [79, 80] because the βI term reduces "ridges" in the cost function $\Psi(x)$. Such ridges are associated with singular vectors of A having small singular values. Chapter 17 discusses such estimators in more detail.

Example 1.7.1 Fig. 1.7.1 shows a random image x, called a gaussian random field (GRF), drawn from the gaussian prior distribution (1.7.4) where $x \sim N(0, I)$.



Figure 1.7.1: Random images drawn from the prior distribution for gaussian random fields (1.7.4) with $\mu_x = 0$. Left: $K_x = I$. Right: $K_x = [C'C]^{-1}$ for the 2D differencing matrix C defined in (1.10.8).

1.7.3.5 Circulant approximation in white gaussian case (Wiener filter)

The MAP estimator (1.7.10), involves a large matrix inverse that may provide little intuition. For insight into the MAP estimator's properties, consider the case where A is circulant, so $A = Q^{-1}\Gamma Q$, where $\Gamma = \text{Diag}\{B_k\}$ and B_k was defined in (1.4.27). In the circulant case with white gaussian noise the MAP estimator (1.7.10), simplifies as follows:

$$\begin{aligned} \hat{\boldsymbol{x}}_{\text{MAP}} &= \left[(\boldsymbol{Q}^{-1}\boldsymbol{\Gamma}\boldsymbol{Q})'(\boldsymbol{Q}^{-1}\boldsymbol{\Gamma}\boldsymbol{Q}) + \beta\sigma^{2}\boldsymbol{I} \right]^{-1} (\boldsymbol{Q}^{-1}\boldsymbol{\Gamma}\boldsymbol{Q})'\boldsymbol{y} \\ &= \left[\boldsymbol{Q}^{-1}\boldsymbol{\Gamma}'\boldsymbol{\Gamma}\boldsymbol{Q} + \beta\sigma^{2}\boldsymbol{Q}^{-1}\boldsymbol{Q} \right]^{-1}\boldsymbol{Q}^{-1}\boldsymbol{\Gamma}'\boldsymbol{Q}\boldsymbol{y} \\ &= \boldsymbol{Q}^{-1} \left[\boldsymbol{\Gamma}'\boldsymbol{\Gamma} + \beta\sigma^{2}\boldsymbol{I} \right]^{-1}\boldsymbol{\Gamma}'\boldsymbol{Q}\boldsymbol{y} = \boldsymbol{Q}^{-1} \operatorname{Diag}\{L_{k}\}\boldsymbol{Q}\boldsymbol{y}. \end{aligned}$$
(1.7.11)

This is just a filter having the following frequency response:

$$L_{k} = \frac{B_{k}^{*}}{|B_{k}|^{2} + \beta\sigma^{2}}.$$
(1.7.12)

This is a DFT-based **Wiener filter** that has the following properties.

- As $\beta \to 0$, this filter approaches the inverse filter $1/B_k$.
- As $\beta \to \infty$, the frequency response of this filter approaches zero.
- A limit of zero is "sensible" because the assumed prior mean is 0; large β corresponds to high prior confidence in that mean, so the MMSE estimation strategy degenerates to the zero estimate.



Figure 1.7.2: Illustration of DFT-based Wiener filter frequency response $L(\Omega)$ for three values of $\beta\sigma^2$.

Fig. 1.7.2 illustrates the properties of this filter for the case $b[n] = \frac{1}{5}\delta[n-1] + \frac{3}{5}\delta[n] + \frac{1}{5}\delta[n+1]$ for which the **DFT coefficients** are $B_k = B(2\pi k/N)$ where the corresponding **DTFT**, defined in (1.4.28), is $B(\Omega) = \frac{3}{5} + \frac{2}{5}\cos\Omega$ and $L_k = L(2\pi k/N)$.

fig_dft_wiene:

.gauss.Lk

Demo See demo_res_wiener.m.

Shrinking the entire estimate down to zero is unnatural for most imaging problems. So apparently the gaussian prior with mean zero and covariance $K_x = (1/\beta)I$ is an unrealistic model for typical real-world images. Although one could certainly improve on this simplistic prior, it is nevertheless quite difficult in general to formulate realistic priors. Therefore, throughout the remainder of this book, we abandon the Bayesian philosophy and focus instead on a close cousin: **penalized-likelihood** estimators. The implementations of MAP methods and penalized-likelihood methods are quite similar, but the the philosophy and terminology differ somewhat. In the end it is something of a matter of personal preference.

1.8 Penalized-likelihood estimation (s,res,stat,pl)

The general form of a MAP estimator (1.7.2) involves maximizing a function that consists of a log-likelihood term that quantifies agreement with the measurements, and another term that quantifies agreement with prior expectations. For the gaussian example (1.7.9) the log-prior was simply proportional to the negative of the **energy** of the signal, *i.e.*, $\log p(x) = -\beta ||x||^2$.

In the framework of **penalized-likelihood** estimation, one also finds the minimizer of a cost function consisting of two terms. Specifically, one finds \hat{x} by minimizing a cost function of the following form:

$$\boldsymbol{x} = \underset{\boldsymbol{x}}{\operatorname{arg\,min}} \Psi(\boldsymbol{x})$$
$$\Psi(\boldsymbol{x}) = -\log p(\boldsymbol{y} \mid \boldsymbol{x}) + \beta R(\boldsymbol{x}). \qquad (1.8.1)$$

The first term is the negative of the log-likelihood, which quantifies the disagreement between x and the measurements y. We would like this term to be small. The second term is a regularizing **penalty function** $R : \mathbb{R}^{n_p} \to \mathbb{R}$ that penalizes an object x according to how much it departs from our assumptions about image properties.

The **regularization parameter** β controls the trade-off between the fit to the data and (typically) the smoothness of \hat{x} . For very small β , \hat{x} will closely fit the data, which usually means very good spatial resolution in the absence of noise, but very noisy estimates in the presence of noise. Conversely, for large β , \hat{x} will emphasize minimizing R(x), which usually means a smooth estimate with low noise. Chapter 2 and Chapter 24 examine this trade-off in more detail.

Choosing the penalty R(x) is an art involving a multitude of trade-offs that are discussed further in Chapter 2. For example, if we expect objects to have small values, then the **energy** penalty

$$\mathsf{R}(\boldsymbol{x}) = \frac{1}{2} \|\boldsymbol{x}\|^2 = \sum_{j=1}^{n_{\rm p}} \frac{1}{2} |x_j|^2 \tag{1.8.2}$$

could be reasonable. (This approach is also known as **Miller regularization** [81].) But in most imaging problems we expect the object to have nonzero energy, so this choice is not the best penalty function.

Why do we need a penalty function in the first place? Because the absence of such a term in the cost function leads again to the "inverse" solution (ML estimate) which greatly amplifies noise and leads to large image oscillations. These oscillations are contrary to our prior expectations about what images look like. So penalty functions that discourage highly oscillatory images usually are more natural than an energy penalty.

A penalty function that discourages high spatial frequency oscillations is called a **roughness penalty**. The simplest type of roughness penalty discourages disparities between neighboring pixel values. It is easiest to first see the effects of such a penalty function in a 1D example, as follows.

s, res, stat, 1d 1.8.1 1D 1st-order roughness penalty

Consider a 1D problem where the elements of $x \in \mathbb{R}^N$ correspond to consecutive "pixel" values $(f[0], \ldots, f[N-1])$. A natural measure of "roughness" of such a signal is the following penalty function that improves somewhat on (1.8.2):

$$\mathsf{R}(\boldsymbol{x}) = \sum_{j=2}^{N} \frac{1}{2} |x_j - x_{j-1}|^2 = \sum_{n=1}^{N-1} \frac{1}{2} |f[n] - f[n-1]|^2, \qquad (1.8.3)$$

using (1.4.7). This penalty function assigns a high cost when neighboring pixel values are very different, thereby discouraging roughness and favoring spatially smooth estimates.

e,res,r

To proceed, it will be convenient to translate this penalty function into a matrix-vector form. Towards that end, consider the following $(N - 1) \times N$ finite differencing matrix:

$$\boldsymbol{C} = \boldsymbol{D}_{N} \triangleq \begin{bmatrix} -1 & 1 & 0 & 0 & \dots & 0 \\ 0 & -1 & 1 & 0 & \dots & 0 \\ & \ddots & \ddots & & \\ 0 & \dots & 0 & -1 & 1 & 0 \\ 0 & \dots & 0 & 0 & -1 & 1 \end{bmatrix}, \text{ so } \boldsymbol{C}\boldsymbol{x} = \begin{bmatrix} x_{2} - x_{1} \\ \vdots \\ x_{N} - x_{N-1} \end{bmatrix}.$$
(1.8.4)

This C is a sparse matrix because most of its elements are zero. (See §2.14.1.3.) With C thus defined, clearly $[Cx]_k = x_{k+1} - x_k$, so

$$\mathsf{R}(\boldsymbol{x}) = \sum_{k=1}^{N-1} \frac{1}{2} \left\| [\boldsymbol{C}\boldsymbol{x}]_k \right\|^2 = \frac{1}{2} \left\| \boldsymbol{C}\boldsymbol{x} \right\|^2 = \frac{1}{2} \boldsymbol{x}' \boldsymbol{C}' \boldsymbol{C} \boldsymbol{x} = \frac{1}{2} \boldsymbol{x}' \mathsf{R} \boldsymbol{x}. \tag{1.8.5}$$

The matrix **R** is the Hessian of the roughness penalty R(x), *i.e.*, the matrix of its second partial derivatives. Here, **R** is the following "nearly Toeplitz" matrix:

$$\mathbf{R} \triangleq \mathbf{C}'\mathbf{C} = \begin{bmatrix} 1 & -1 & 0 & \dots & 0 & 0 \\ -1 & 2 & -1 & 0 & \dots & 0 \\ & & \ddots & \ddots & \ddots & \\ 0 & \dots & 0 & -1 & 2 & -1 \\ 0 & 0 & \dots & 0 & -1 & 1 \end{bmatrix}.$$
 (1.8.6)

This type of penalty function is called a **quadratic penalty** because R(x) is a quadratic form in x. The quadratic form is particularly convenient when the measurements have gaussian distributions. See [82] for analysis of the eigenvalues and eigenvectors of (1.8.6) for various boundary conditions including Neumann boundary conditions and Dirichlet boundary conditions.

Often it is expected that f[n] is zero near the ends of its support, such as in 2D tomography problems where there is usually "black air space" surrounding the body. In such case, an alternate penalty function is

$$\mathsf{R}(\boldsymbol{x}) = \frac{1}{2} |f[0] - 0|^2 + \frac{1}{2} |f[N-1] - 0|^2 + \sum_{n=1}^{N-1} \frac{1}{2} |f[n] - f[n-1]|^2.$$

In this case, the form $R(x) = \frac{1}{2} \|Cx\|^2$ in (1.8.5) still applies, but here the $(N+1) \times N$ differencing matrix C has the following form:

$$C = \begin{bmatrix} 1 & 0 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots \\ & D_N & & \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & 0 & 1 \end{bmatrix},$$
(1.8.7)

where D_N was defined in (1.8.4). The Hessian $\mathbf{R} = C'C$ for this penalty is *exactly* Toeplitz with elements

$$R_{kj} = 2\,\delta[k-j] - \delta[k-j-1] - \delta[k-j+1]\,.$$

Having a constant diagonal simplifies slightly the implementation of iterative algorithms that use diagonal preconditioners.

1.8.2 Linear gaussian case: QPWLS estimator

Combining the log-likelihood corresponding to the linear gaussian case (1.7.3) with the preceding quadratic penalty function (1.8.5) yields the following cost function for penalized-likelihood estimation:

$$\Psi(\boldsymbol{x}) = \frac{1}{2} (\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x})' \boldsymbol{K}_{\varepsilon}^{-1} (\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}) + \beta \frac{1}{2} \boldsymbol{x}' \boldsymbol{R} \boldsymbol{x}.$$
(1.8.8)

By similar analysis as in §1.7.3.1, the minimizer¹¹ of $\Psi(x)$ is

$$\hat{\boldsymbol{x}} = \left[\boldsymbol{A}'\boldsymbol{K}_{\varepsilon}^{-1}\boldsymbol{A} + \beta\boldsymbol{\mathsf{R}}\right]^{-1}\boldsymbol{A}'\boldsymbol{K}_{\varepsilon}^{-1}\boldsymbol{y}.$$
(1.8.9)

This regularized solution dates back at least to [83, eqn. (7)] and it is simply a special case of the MAP estimator (1.7.6), where $\mu_x = 0$ and $\beta \mathbf{R} = K_x^{-1}$. In Bayesian language, the penalty function (1.8.3) corresponds to the following improper gaussian prior:

$$\mathbf{p}(\boldsymbol{x}) = c \,\mathrm{e}^{-\beta \,\frac{1}{2} \boldsymbol{x}' \mathbf{R} \boldsymbol{x}} \,. \tag{1.8.10}$$

This is an **improper prior** or **degenerate** normal distribution because the **R** in (1.8.6) above is not invertible. Indeed most useful quadratic penalty functions have singular Hessians, a property that is entirely acceptable in penalized-likelihood estimation but is perhaps somewhat awkward for a **Bayesian** interpretation.

We refer to (1.8.8) and (1.8.9) as a quadratically penalized weighted least-squares (**QPWLS**) estimator.

circ 1.8.3 Circulant analysis of QPWLS restoration

For further insight into the properties of the QPWLS estimator (1.8.9), it is again convenient to apply circulant approximations.

First we observe that in typical tomographic imaging applications the object usually does not fill the entire field of view (think of the "black air space" around the head in a brain scan). So we alter the form of R(x) to make it a circular shift-invariant functional by analyzing the following roughness penalty function:

$$\mathsf{R}(\boldsymbol{x}) = \frac{1}{2} \left| x_1 - x_N \right|^2 + \sum_{j=2}^{N} \frac{1}{2} \left| x_j - x_{j-1} \right|^2. \tag{1.8.11}$$

The initial term is needed for analysis only and is rarely implemented in practice.

To put this penalty function in matrix-vector form, consider the following $N \times N$ modified C matrix:

$$\boldsymbol{C} = \begin{bmatrix} -1 & 1 & 0 & \dots & 0 \\ 0 & -1 & 1 & \dots & 0 \\ & & \ddots & \ddots & \\ 0 & \dots & 0 & -1 & 1 \\ 1 & 0 & \dots & 0 & -1 \end{bmatrix}, \text{ where } \boldsymbol{C}\boldsymbol{x} = \begin{bmatrix} x_2 - x_1 \\ \vdots \\ x_N - x_{N-1} \\ x_1 - x_N \end{bmatrix}.$$
(1.8.12)

This C matrix again satisfies (1.8.5) for the preceding R(x), where now **R** is the following circulant matrix¹²

$$\mathbf{R} \triangleq \mathbf{C}'\mathbf{C} = \begin{bmatrix} 2 & -1 & 0 & \dots & 0 & -1 \\ -1 & 2 & -1 & 0 & \dots & 0 \\ & & \ddots & \ddots & \ddots & \\ 0 & \dots & 0 & -1 & 2 & -1 \\ -1 & 0 & \dots & 0 & -1 & 2 \end{bmatrix}.$$
 (1.8.13)

Because **R** is circulant, it is diagonalized by the DFT matrix Q^{-1} , *i.e.*, **R** = $Q^{-1}\Pi Q$ where Π is diagonal with entries R_k . In particular, evaluating the DFT of the first column of this **R** shows that its eigenvalues (DFT coefficients) are¹³

$$\mathsf{R}_{k} = 2 - \mathrm{e}^{-i2\pi k/N} - \mathrm{e}^{i2\pi k/N} = 2 - 2\cos(2\pi k/N).$$
(1.8.14)

Suppose further that the system matrix A is also circulant, *i.e.*, $A = Q^{-1}\Gamma Q$, and that the noise is white: $K_{\varepsilon} = \sigma^2 I$. Substituting these assumptions into the QPWLS estimator (1.8.9) yields

$$\hat{\boldsymbol{x}} = \operatorname*{arg\,min}_{\boldsymbol{x}} \Psi(\boldsymbol{x}) = \left[\boldsymbol{A}' \boldsymbol{A} + \beta \sigma^2 \boldsymbol{\mathsf{R}}
ight]^{-1} \boldsymbol{A}' \boldsymbol{y}$$

¹²To realize how special this matrix is, see http://www.siam.org/news/news.php?id=1697.

e, res, xh, qpwls

e, res, stat, pl, eRk

f,eig,R

¹¹One must address the invertibility of $\mathbf{A}' \mathbf{K}_{\varepsilon}^{-1} \mathbf{A} + \beta \mathbf{R}$ in (1.8.9), because in general $\mathbf{A}' \mathbf{K}_{\varepsilon}^{-1} \mathbf{A}$ and \mathbf{R} are each only positive semidefinite. For penalty functions based on first-order differences, like (1.8.3) and (1.10.1), the null space of \mathbf{R} is spanned by 1, the vector of all ones. For most imaging systems, $\mathbf{A1} \neq \mathbf{0}$, so the null spaces of $\mathbf{A}' \mathbf{K}_{\varepsilon}^{-1} \mathbf{A}$ and \mathbf{R} are disjoint. For such systems, their sum is invertible.

¹³ For the special case of the first-order roughness penalty (1.8.3), one can determine its eigenvalues and eigenvectors exactly without imposing the circulant model, *e.g.*, [84]. The eigenvalues of (1.8.6) are $R_k = 2-2\cos(\pi k/N)$, k = 0, ..., N-1. Nevertheless, the circulant approximation provides more intuition because of its frequency response interpretation.

$$= Q^{-1} \left[\boldsymbol{\Gamma}' \boldsymbol{\Gamma} + \beta \sigma^2 \boldsymbol{\Pi} \right]^{-1} \boldsymbol{\Gamma}' Q \boldsymbol{y} = Q^{-1} \operatorname{Diag}\{L_k\} Q \boldsymbol{y}.$$
(1.8.15)

So once again our estimator \hat{x} is a linear, circularly shift-invariant, Wiener-like filter¹⁴ with frequency response

$$L_{k} = \frac{B_{k}^{*}}{|B_{k}|^{2} + \beta \sigma^{2} \mathsf{R}_{k}}.$$
(1.8.16)

Again, as $\beta \to 0$, this filter approaches the inverse filter: $L_k \to 1/B_k$. This property is inherent to the form (1.8.1). However, because $R_0 = 0$, as $\beta \to \infty$, we have the following:

$$L_k \rightarrow \begin{cases} 1/B_0, & k=0\\ 0, & \text{otherwise.} \end{cases}$$

This behavior is preferable to that of the energy penalty (1.8.2) because at least the DC term (k = 0) is unaffected by the regularizing penalty function (1.8.11).

Example 1.8.1 *Fig. 1.8.1 illustrates these properties for the same example considered in Fig. 1.7.2. As desired, the QPWLS filter response at low frequencies is nearly unity here, unlike in Fig. 1.7.2.*



x,res,stat,lpl,gaus



Figure 1.8.1: Illustration of properties of the Wiener-like filter (1.8.16) corresponding to QPWLS estimation for 1D signal restoration example.

1.8.4 Discussion

Although the roughness penalty function (1.8.3) yields behavior that is preferable to the energy penalty function (1.8.2), it still yields a linear method that is essentially a lowpass filter, so we can reduce noise only by compromising spatial resolution. This is a fundamental **resolution-noise trade-off** in all (linear) imaging systems and image processing methods. This trade-off can be overcome only by considering nonlinear estimators. Nonquadratic penalty functions can smooth noise while preserving image edges so are a focus of the algorithms discussed in this *book*. However, being nonlinear they are less amenable to the types of "signal processing" analysis described above.

As discussed in Chapter 24, in certain imaging problems it can be desirable to formulate a penalty function R(x) that *depends on the measurements* y, *e.g.*, [86–88]. Such formulations are perfectly compatible with the penalized-likelihood philosophy, but seem at odds with the Bayesian notion of a "prior." This is another reason why we prefer the former philosophy.

[RQ5]

¹⁴Technically speaking the term Wiener filter is a Bayesian concept because it was derived originally using a prior model for the object \boldsymbol{x} . In image restoration, the traditional non-Bayesian term for this approach is **constrained least-squares** [85]. Here we treat $R(\boldsymbol{x})$ as a penalty function rather than as a constraint.

1.9 Mean and variance analysis (resolution-noise trade-offs) (s,res,pl,mav1)

For further insight into the **resolution-noise trade-off** associated with penalized-likelihood estimation, this section analyzes the first two moments of the 1D linear QPWLS estimator \hat{x} in (1.8.15). Chapter 24 and Chapter 25 consider more complicated nonlinear problems. Ideally we would analyze the entire statistical behavior of an estimator \hat{x} by studying its probability distribution $p(\hat{x})$. Unfortunately, for nonlinear estimators such analysis is intractable except in some special cases, *e.g.*, [89]. Therefore, we focus on the first two moments of \hat{x} , or, in nonlinear cases, the approximations thereof.

The QPWLS estimator \hat{x} in (1.8.15) is linear, and we can write it as $\hat{x} = Ly$ where

$$\boldsymbol{L} \triangleq \left[\boldsymbol{A}'\boldsymbol{K}_{\boldsymbol{\varepsilon}}^{-1}\boldsymbol{A} + \beta \boldsymbol{\mathsf{R}}\right]^{-1}\boldsymbol{A}'\boldsymbol{K}_{\boldsymbol{\varepsilon}}^{-1} = \boldsymbol{Q}^{-1}\left[\boldsymbol{\Gamma}'\boldsymbol{\Gamma} + \beta \sigma^2 \boldsymbol{\mathsf{\Pi}}\right]^{-1}\boldsymbol{\Gamma}'\boldsymbol{Q}.$$

Recall that $y = Ax + \varepsilon$ where $\varepsilon \sim N(0, \sigma^2 I)$, so E[y | x] = Ax and $K_{\varepsilon} = Cov\{y | x\} = \sigma^2 I$. Thus, by the linearity of expectation, the mean of \hat{x} for a given x is

$$\mathsf{E}[\hat{\boldsymbol{x}} \mid \boldsymbol{x}] = \mathsf{E}[\boldsymbol{L}\boldsymbol{y} \mid \boldsymbol{x}] = \boldsymbol{L} \,\mathsf{E}[\boldsymbol{y} \mid \boldsymbol{x}] = \boldsymbol{L}\boldsymbol{A}\boldsymbol{x} = \left[\boldsymbol{A}'\boldsymbol{A} + \beta\sigma^2\boldsymbol{\mathsf{R}}\right]^{-1}\boldsymbol{A}'\boldsymbol{A}\boldsymbol{x}$$
$$= \boldsymbol{Q}^{-1}\left[\boldsymbol{\Gamma}'\boldsymbol{\Gamma} + \beta\sigma^2\boldsymbol{\mathsf{\Pi}}\right]^{-1}\boldsymbol{\Gamma}'\boldsymbol{\Gamma}\boldsymbol{Q}\boldsymbol{x} = \boldsymbol{Q}^{-1}\,\mathsf{Diag}\{M_k\}\,\boldsymbol{Q}\boldsymbol{x}.$$
(1.9.1)

So the expectation of \hat{x} is simply a filtered version of the true object x with filter frequency response

$$M_{k} = \frac{|B_{k}|^{2}}{|B_{k}|^{2} + \beta\sigma^{2}\mathsf{R}_{k}} = L_{k}B_{k}, \qquad (1.9.2)$$

because $\Gamma = \text{Diag}\{B_k\}$ and $\Pi = \text{Diag}\{\mathsf{R}_k\}$, where L_k was defined in (1.8.16). For good spatial resolution, we would like this "filter" to pass all spatial frequencies with a gain of unity, which means we would like $\beta \mathsf{R}_k$ to be small.

To analyze the covariance of \hat{x} , we use the following particularly important property of covariance matrices:

$$\operatorname{Cov}\{Lz\} = L\operatorname{Cov}\{z\}L', \tag{1.9.3}$$

which follows directly from the definition (1.6.2). Thus the covariance of \hat{x} for a given true object x is:

$$\operatorname{Cov}\{\hat{\boldsymbol{x}} \mid \boldsymbol{x}\} = \operatorname{Cov}\{\boldsymbol{L}\boldsymbol{y} \mid \boldsymbol{x}\} = \boldsymbol{L}\operatorname{Cov}\{\boldsymbol{y} \mid \boldsymbol{x}\}\boldsymbol{L}' = \boldsymbol{L}(\sigma^{2}\boldsymbol{I})\boldsymbol{L}'$$
$$= \sigma^{2}\left[\boldsymbol{A}'\boldsymbol{A} + \beta\sigma^{2}\boldsymbol{R}\right]^{-1}\boldsymbol{A}'\boldsymbol{A}\left[\boldsymbol{A}'\boldsymbol{A} + \beta\sigma^{2}\boldsymbol{R}\right]^{-1}.$$
(1.9.4)

This matrix expression may not be particularly intuitive, so again we consider the circulant model (1.4.31). Then the covariance simplifies as follows:

$$\operatorname{Cov}\{\hat{\boldsymbol{x}} \mid \boldsymbol{x}\} = \sigma^2 Q^{-1} \left[\boldsymbol{\Gamma}' \boldsymbol{\Gamma} + \beta \sigma^2 \boldsymbol{\Pi} \right]^{-1} \boldsymbol{\Gamma}' \boldsymbol{\Gamma} \left[\boldsymbol{\Gamma}' \boldsymbol{\Gamma} + \beta \sigma^2 \boldsymbol{\Pi} \right]^{-1} Q$$
$$= Q^{-1} \operatorname{Diag}\{P_k\} Q, \qquad (1.9.5)$$

where the following diagonal entries correspond to the **noise power spectrum** (NPS) of the estimator \hat{x} :

$$P_{k} \triangleq \frac{\sigma^{2} |B_{k}|^{2}}{\left(|B_{k}|^{2} + \beta \sigma^{2} \mathsf{R}_{k}\right)^{2}} = \sigma^{2} |L_{k}|^{2}.$$
(1.9.6)

For a low-noise restoration, we would like the variance of \hat{x}_i to be small. The variance of \hat{x}_i is given by

$$\begin{aligned} \operatorname{Var}\{\hat{x}_{j} \mid \boldsymbol{x}\} &= \boldsymbol{e}_{j}^{\prime} \operatorname{Cov}\{\hat{\boldsymbol{x}} \mid \boldsymbol{x}\} \boldsymbol{e}_{j} = \boldsymbol{e}_{j}^{\prime} \boldsymbol{Q}^{-1} \operatorname{Diag}\{P_{k}\} \boldsymbol{Q} \boldsymbol{e}_{j} \\ &= \frac{1}{N} \sum_{k=0}^{N-1} P_{k} = \frac{\sigma^{2}}{N} \sum_{k=0}^{N-1} |L_{k}|^{2}, \end{aligned}$$
(1.9.7)

because the DFT of a Kronecker impulse is unity, *i.e.*, $|Qe_j|_k = 1$, and we use (1.4.30). In 2D the factor $\frac{\sigma^2}{N}$ is $\frac{\sigma^2}{MN}$. Reducing image noise is equivalent to having a low variance. From (1.9.6) and (1.9.7), having a small variance requires βR_k to be large whenever B_k is small.

Comparing (1.9.2) and (1.9.7) illustrates succinctly the fundamental **resolution-noise trade-off** in any linear image restoration method. For good spatial resolution, we want (1.9.2) to be approximately unity, which means $\beta R_k \approx 0$, but for low noise, (1.9.7) requires that βR_k be large.

e,res,pl,mear

e,res,pl,nps

As a concrete example, consider the **image denoising** problem where the system impulse response in (1.2.3) is $b[n] = \delta[n]$, so $B_k = 1$. If $\beta = 1$ and $\sigma^2 = 1$, then (1.9.2) gives $\frac{1}{1+R}$ whereas (1.9.7) gives $\frac{1}{(1+R)^2}$. We cannot simultaneously make the first equation near unity and the second equation near 0. Consequently, if we use a nonzero R to reduce noise, we will also reduce high spatial frequencies. The principal visual effect of this attenuation will be blurring of edges in the image.

The origin of this undesirable trade-off is the quadratic roughness penalty function itself. In Bayesian terms, a quadratic roughness penalty corresponds to a gaussian prior, yet most real world images are not particularly gaussian. To overcome this limitation we will consider nonlinear methods based on nonquadratic penalty functions. But first we consider how to form roughness penalties for 2D images.

Fig. 1.9.1 illustrates this trade-off by showing the overall frequency response M_k in (1.9.2) and noise power spectrum P_k in (1.9.6) for three values of the regularization parameter β . As β decreases, M_k improves towards unity, but P_k increases.



Figure 1.9.1: Illustration of trade-off between spatial resolution (over all frequency response) and noise power spec- $_{fig_res_wiener_np}$ trum in image restoration with a quadratic roughness penalty, for three values of the regularization parameter β .

Demo See demo_res_wiener.m.

[RQ6]

1.10 Roughness penalties in 2D (s,res,penal2)

Thus far we have considered only the simple 1D roughness penalty of the form (1.8.3). Applying penalized-likelihood methods to image restoration problems requires 2D roughness penalty functions.

1.10.1 Quadratic regularization

Extrapolating (1.8.3) from 1D signals to 2D objects f[m, n] suggests the following simple roughness penalty:

$$\mathsf{R}(f) = \sum_{m=1}^{M-1} \sum_{n=0}^{N-1} \frac{1}{2} \left| f[m,n] - f[m-1,n] \right|^2 + \sum_{m=0}^{M-1} \sum_{n=1}^{N-1} \frac{1}{2} \left| f[m,n] - f[m,n-1] \right|^2.$$
(1.10.1)

This quadratic penalty function discourages disparities between horizontal and vertical neighboring pixels. For 2D roughness penalty functions, it is often useful to include *diagonal* neighboring pixels, *i.e.*, to include terms of the form $|f[m, n] - f[m - 1, n - 1]|^2$ for example. See §2.3 for further generalizations.

The notation in (1.10.1) becomes even more cumbersome in 3D, particularly as one uses more neighbors. For a more concise expression, write the penalty function in terms of the vector x instead of the 2D array f[m, n], recalling (1.4.16), as follows:

$$\mathsf{R}(\boldsymbol{x}) = \sum_{j=1}^{n_{\rm p}} \sum_{l \in \mathcal{N}_j} \frac{1}{2} |x_j - x_l|^2, \qquad (1.10.2)$$

where N_j denotes the set of neighbors of the *j*th pixel, or more precisely, half of that set of neighbors. For a $M \times N$ object, a **first-order neighborhood** means¹⁵

$$\mathcal{N}_j = \{j - 1, \, j - M\} \tag{1.10.3}$$

and a **2nd-order neighborhood** means

$$\mathcal{N}_j = \{j - 1, j - M, j - M - 1, j - M + 1\}$$

To help understand these sets, the following diagram illustrates the distinction between 2D pixel coordinates and 1D vector element indexes of lexicographically ordered arrays for a 3×3 neighborhood in a $M \times N$ image.

1D indexes				2	D coordinate			
j - M - 1	j - M	j - M + 1		[m-1, n-1]	[m, n-1]	[m+1, n-1]	$\rightarrow m$	e, res, penal2, j, m, n (1 10 4)
j-1	j	j+1		[m-1,n]	[m,n]	[m+1, n]	\hat{n}	(1.10.4)
j+M-1	j + M	j + M + 1		[m-1, n+1]	[m, n+1]	[m+1, n+1]		

Again, an appropriate matrix-vector representation can further greatly simplify notation. Each term in (1.10.1) or (1.10.2) involves a difference of nearby pixel values, *e.g.*, $x_j - x_l$, which is a simple linear combination. For a first-order neighborhood, the 2D roughness penalty (1.10.2) has the following concise matrix-vector form:

$$\mathsf{R}(\boldsymbol{x}) = \frac{1}{2} \|\boldsymbol{C}_{1}\boldsymbol{x}\|^{2} + \frac{1}{2} \|\boldsymbol{C}_{2}\boldsymbol{x}\|^{2}, \qquad (1.10.5)^{\text{e, res, penal2, Rx, hv}}$$

provided we define appropriately the matrices C_1 and C_2 . Each row of C_1 corresponds to one term in the first summation in (1.10.1). The natural choice for C_1 would have size $(M - 1)N \times MN$, because this is the number of terms in the first sum in (1.10.1). However, it can be more convenient for implementation to choose C_1 and C_2 to both have size $MN \times MN$, allowing each matrix to have a few rows that are entirely zero. Such zero rows do not change the value of the penalty function. (Instead of being entirely zero, those rows could have entries that correspond to other end conditions.) See Fig. 1.10.1 and Problem 1.14.

Recalling (1.4.16), we can identify the term f[m, n] - f[m - 1, n] with the kth row of C_1 , where k = 1 + m + nM. With this natural ordering, the elements of C_1 are as follows:

$$[\mathbf{C}_{1}]_{kj} = \begin{cases} 1, & k = j = 1 + m + nM \\ -1, & k = 1 + m + nM, \ j = k - 1 \\ 0, & \text{otherwise}, \end{cases}$$
(1.10.6)

e.res.penal2.Ni.]

 $^{^{15}(1.10.3)}$ must be modified slightly when the *j*th pixel is on the left or top border of the image.

for m = 1, ..., M - 1, n = 0, ..., N - 1, *i.e.*, for $k = 2, ..., n_p = MN$. Each nonzero row of C_1 has a single "-1" entry and a "1" entry, and all other elements are zero. Thus C_1 is a very sparse matrix. One can define C_2 similarly. (See §2.3.) One can verify that if x denotes the lexicographic representation of f[m, n] per (1.4.14), then

$$[\mathbf{C}_1 \mathbf{x}]_k \Big|_{k=1+m+nM} = \begin{cases} f[m,n] - f[m-1,n], & m = 1, \dots, M-1 \\ 0, & n = 0, \dots, N-1 \\ 0, & \text{otherwise.} \end{cases}$$

We can write the quadratic roughness penalty (1.10.5) even more concisely as follows:

$$\mathsf{R}(\boldsymbol{x}) = \frac{1}{2} \|\boldsymbol{C}\boldsymbol{x}\|^2,$$
 (1.10.7)

by defining the following $2MN \times MN$ matrix

$$\boldsymbol{C} = \begin{bmatrix} \boldsymbol{C}_1 \\ \boldsymbol{C}_2 \end{bmatrix}. \tag{1.10.8}$$

See Chapter 2 for extensions and details about implementing such C matrices.

Fig. 1.10.1 illustrates C_1 and C_2 in (1.10.8) for a small 2D image. Each matrix has $N \times N$ blocks of $M \times M$ elements. Likewise, Fig. 1.10.2 shows the case where we use periodic boundary conditions. In this latter case, both C_1 and C_2 are block circulant with circulant blocks (BCCB).



Figure 1.10.1: Illustration of finite-differencing matrices C_1 and C_2 for a 2D image with M = 5 and N = 4. There are $N \times N$ blocks each of size $M \times M$.

The Hessian of the quadratic regularizer (1.10.7) is $\mathbf{R} = \nabla^2 \mathbf{R} = C'_1 C_1 + C'_2 C_2$. Fig. 1.10.3 illustrates this Hessian for the case of periodic boundary conditions, for which **R** is BCCB. Following the analysis in §1.4.3.2, the eigenvalues of this **R** correspond to the 2D DFT of the (suitably reshaped) first column of **R**. That first column, when reshaped, corresponds to the impulse response

$$r[m,n] = 4\,\delta[m]\,\delta[n] - \delta[m-1]\,\delta[n] - \delta[m+1]\,\delta[n] - \delta[m]\,\delta[n-1] - \delta[m]\,\delta[n+1]$$

which has corresponding 2D DFT

$$\left\{4-2\cos\left(\frac{2\pi}{M}k\right)-2\cos\left(\frac{2\pi}{N}l\right): k=0,\ldots,M-1, \ l=0,\ldots,N-1\right\},\$$

and these are the MN eigenvalues of **R**. See Problem 1.16.

Example 1.10.1 As discussed in §1.8.2, using a penalty function of the form (1.10.7) is equivalent to a gaussian prior model of the form (1.8.10) in a Bayesian formulation. Fig. 1.7.1 shows an example of a random image (a gaussian random field) drawn from this "prior," having covariance $K_x = \mathbb{R}^{-1}$, where $\mathbb{R} = C'C$. This matrix is not quite invertible, so Fig. 1.7.1 used the pseudoinverse of a circulant approximation to \mathbb{R} . See Problem 1.28.

fig res c21



Figure 1.10.2: Illustration of finite-differencing matrices C_1 and C_2 for a 2D image with M = 5 and N = 4 for the case of periodic boundary conditions.



Figure 1.10.3: Illustration of quadratic regularizer Hessian $\mathbf{R} = C'_1 C_1 + C'_2 C_2$ for a 2D image with M = 5 and N = 4 for the case of periodic boundary conditions. This Hessian matrix is **BCCB**.

1.10.2 Nonquadratic (edge preserving) regularization

As discussed in §1.9, a quadratic roughness penalty causes blurring of object edges, because squaring the differences between neighboring pixels strongly encourages neighboring values to be similar. To try to preserve edges, we can replace the quadratic function¹⁶ $\psi(z) = \frac{1}{2} |z|^2$ in (1.10.1) with a nonquadratic function ψ that rises less rapidly than the quadratic when the difference $|x_j - x_k|$ exceeds some user-selected threshold $\delta > 0$. One way to avoid over-regularizing the differences between neighboring pixels is to use the Huber function illustrated in Fig. 1.10.4:

$$\psi(z) = \psi_{\delta}(z) \triangleq \begin{cases} \frac{1}{2} |z|^2, & |z| \le \delta \\ \delta |z| - \frac{1}{2} \delta^2, & |z| > \delta \end{cases} = \delta^2 \psi_1(z/\delta) .$$

$$(1.10.9)^{\circ}$$

Often such **edge preserving** potential functions are quadratic near zero, but roughly linear far from zero. Large disparities between neighboring pixels, such as might arise near object edges, are penalized less by such a **potential function**¹⁷ than by quadratic penalty functions. (See §1.10.3.)

It is possible to use different potential functions for different spatial locations. Therefore, most of the algorithms described in this *book* are derived for roughness penalty functions having the following general form:

$$\mathsf{R}(\boldsymbol{x}) = \sum_{k=1}^{K} \psi_k([\boldsymbol{C}\boldsymbol{x}]_k), \qquad (1.10.10)$$

where $[Cx]_k = \sum_{j=1}^{n_p} c_{kj} x_j$. The matrix C is $K \times n_p$ where $n_p = MN$, and for the simple 2D case (1.10.1) with horizontal and vertical neighbors, we have K = 2MN. This form is sufficiently general to represent many, but not all, regularizers (and log priors) that have been described in the literature. §2.7 describes many other choices for ψ_k .



Figure 1.10.4: Illustration of some potential functions ψ used for regularization: the quadratic function, the Huber function, and the "broken-parabola" function (see §1.13.1).

fig_broker

1.10.3 Analysis of least-squares with nonquadratic regularization (s,res,npls)

Although analysis of the properties of penalized-likelihood estimates \hat{x} is more difficult when the regularizer is nonquadratic, we can still get some insight into the edge-preserving characteristics by deriving a recursive expression for \hat{x} as shown in this section.

We focus on penalized least-squares cost functions of the form

$$\Psi(\boldsymbol{x}) = \frac{1}{2} \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}\|^2 + \beta \operatorname{R}(\boldsymbol{x})$$
(1.10.11)

where the penalty function has the general form (1.10.10) but with $\psi_k = \psi$. In (1.10.11) we have dropped the noise variance σ^2 from (1.7.9) because it often is unknown and we can always absorb into β anyway. We will not consider circulant approximations here because nonquadratic penalty functions introduce local shift-variant effects.

For the analysis in this section, we assume the **potential function** ψ satisfies the following two conditions.

¹⁶I use the letter z as the argument of the potential function $\psi(z)$ because the regularizer encourages its argument to be close to zero.

¹⁷The term **potential function** for ψ is prevalent in the Bayesian restoration literature, but originates even earlier in physics literature on the energy of various configurations of spatial models.

- ψ is everywhere differentiable with derivative ψ .
- The following weighting function [90, p. 179] is defined (finite) and nonnegative for all $z \in \mathbb{R}$:

$$\omega_{\psi}(z) \triangleq \frac{\dot{\psi}(z)}{z}.$$
(1.10.12)

For later algorithm derivations and convergence analysis (cf. §14.5.4 and [91]) we will make stronger assumptions about ψ , but these two conditions suffice here. Fig. 1.10.5 illustrates the weighting functions ω_{ψ} for the potential functions shown in Fig. 1.10.4. (Fig. 2.7.1 illustrates many more from Table 2.1.) As detailed in §2.7, usually $\omega_{\psi}(z)$ is a decreasing function of |z|.



Figure 1.10.5: The potential weighting functions $\omega_{\psi}(z)$ for a quadratic potential, Huber potential, and a broken $fig_{res_wpot_huber}$ parabola potential, illustrated using $\delta = 1$.

Typical edge-preserving potential functions have the property that they are nearly quadratic near zero, and nearly linear when the argument exceeds δ . The parameter δ controls the transition between smoothing and edge-preservation, so one must have in advance a rough idea of the anticipated differences between neighboring pixels that straddle region boundaries, or use trial and error to find δ . As elaborated below, the nonquadratic property will encourage most neighboring pixel values to be similar, but will also allow them to be different in image locations where there are sufficient discrepancies between neighbors, *i.e.*, near object edges.

To explore the properties further, first we examine the column gradient of the penalty function:

$$\nabla \mathsf{R}(\boldsymbol{x}) = \sum_{k=1}^{K} \nabla \psi(\boldsymbol{c}'_{k}\boldsymbol{x}) = \sum_{k=1}^{K} \boldsymbol{c}_{k} \, \dot{\psi}([\boldsymbol{C}\boldsymbol{x}]_{k}) = \sum_{k=1}^{K} \boldsymbol{c}_{k} \, \omega_{\psi}([\boldsymbol{C}\boldsymbol{x}]_{k})[\boldsymbol{C}\boldsymbol{x}]_{k} = \boldsymbol{C}' \, \boldsymbol{D}(\boldsymbol{x}) \, \boldsymbol{C}\boldsymbol{x}$$
(1.10.13)

where $c'_k = e'_k C$ denotes the kth row of C and we define the following x-dependent, $K \times K$ diagonal weighting matrix:

$$\boldsymbol{D}(\boldsymbol{x}) \triangleq \mathsf{Diag}\{\omega_{\psi}([\boldsymbol{C}\boldsymbol{x}]_{k})\}.$$
(1.10.14)

(The weighting function (1.10.12) was constructed to enable the final form (1.10.13).) Thus the gradient of the cost function (1.10.11) is

$$\nabla \Psi(\boldsymbol{x}) = -\boldsymbol{A}' \left(\boldsymbol{y} - \boldsymbol{A} \boldsymbol{x} \right) + \beta \boldsymbol{C}' \boldsymbol{D}(\boldsymbol{x}) \boldsymbol{C} \boldsymbol{x}, \qquad (1.10.15)$$

which equated to zero yields

$$oldsymbol{A}'oldsymbol{y} = oldsymbol{A}'A\,\hat{oldsymbol{x}} + etaoldsymbol{C}'\,oldsymbol{D}(\hat{oldsymbol{x}})\,oldsymbol{C}\,\hat{oldsymbol{x}}$$
 .

Rearranging yields the following recursive expression for the estimator \hat{x} :

$$\hat{x} = [A'A + \beta C' D(\hat{x}) C]^{-1} A' y.$$
 (1.10.16)

e.res.npls.wpot

e,res,npls,xh

This is a somewhat remarkable expression, but it is not quite in closed form because \hat{x} is present on the right-hand side. Nevertheless, it provides insight into the properties of nonquadratic penalty functions. (A closed form is known for the 1D case with ideal step-function data for the Huber potential function [92].)

First reconsider the quadratic case where $\psi(z) = z^2/2$. Then $\omega_{\psi}(z) = 1$ so $D(\hat{x}) = I$ and we are back to the usual quadratic penalized least-squares estimator (1.8.9) with its edge-blurring properties.

For more insight into (1.10.16), consider again the 1D problem described in §1.8.1. If we knew where the edges were, we would use a *spatially weighted* penalty function [93]

$$\mathsf{R}(\boldsymbol{x}) = \sum_{j=2}^{N} w_j \, \psi(x_j - x_{j-1}) \tag{1.10.17}$$

where we would set $w_j = 0$ between pixels straddling an edge, and $w_j = 1$ for pixels in relatively uniform regions. This would provide smoothing and hence noise reduction in uniform regions without causing regularization-induced blurring across edges. In the quadratic case where $\psi(z) = z^2/2$, this "oracle weighted" regularizer would lead to the solution

$$\hat{oldsymbol{x}} = \left[oldsymbol{A}' oldsymbol{A} + eta oldsymbol{C}' \operatorname{\mathsf{Diag}}\{w_j\} oldsymbol{C}
ight]^{-1} oldsymbol{A}' oldsymbol{y},$$

which would provide ideal edge-preserving restoration. However, in practice we (usually) do not know where the edges are in advance, so we must "let the algorithm find them." Comparing this expression to (1.10.16), we see that the "only" difference is that in (1.10.16) the weights ω_{ψ} depend on the estimate \hat{x} .

For example, consider the Huber **potential function** given in Table 2.1 and its corresponding **weighting function** shown in Fig. 1.10.5. When the difference $[C \hat{x}]_k$ between neighboring pixels exceeds δ , the corresponding weight is reduced from unity by ω_{ψ} , thereby approximating the effect described in (1.10.17). In other words, instead of needing to know the edge locations in advance, a nonquadratic penalty function can provide *estimate-based* weighting. (See Example 1.11.3 and Fig. 1.11.2 for an example.) In the **denoising** case where A = I, one can think of \hat{x} as an iterative form of adaptive smoothing.

There are explicitly adaptive methods for image restoration where one processes the image y to attempt to locate edge regions, *e.g.*, by using local statistics [94–99]. Such methods are applicable to image restoration problems where y is already an image, but not to other inverse problems such as tomography where y is not an image.

1.11 Minimization algorithms (s,res,alg.tex)

Typically closed-form solutions are unavailable for the minimizer \hat{x} of the cost functions (1.8.1) of interest in inverse problems, so finding \hat{x} requires iterative optimization algorithms. Chapters 11 - 14 describe such algorithms in detail; here we preview just two.

An **iterative algorithm** is a procedure that starts with an initial guess $x^{(0)}$ for \hat{x} , and then recursively generates a sequence¹⁸ $x^{(1)}, x^{(2)}, \ldots$, also denoted $\{x^{(n)}\}$. Ideally, the iterates $\{x^{(n)}\}$ should rapidly approach the minimizer \hat{x} .

1.11.1 Gradient-based algorithms

Most algorithms involve the gradient of the cost function $\Psi(\mathbf{x})$, as described in detail in Chapter 11, Many of the algorithms reduce to the following form:

$$\boldsymbol{x}^{(n+1)} = \boldsymbol{x}^{(n)} - \alpha_n \boldsymbol{D} \, \boldsymbol{\nabla} \Psi(\boldsymbol{x}^{(n)}), \tag{1.11.1}$$

where D is some diagonal preconditioning matrix, and α_n is a step size that affects the convergence rate of the sequence $\{x^{(n)}\}$. Such an algorithm will be of limited use unless it converges to the solution \hat{x} . To preview the convergence analyses described in later chapters, consider the case where $\Psi(x)$ is quadratic, such as in (1.7.5). Such functions can also be written in the following two forms:

$$\Psi(\boldsymbol{x}) = c - \boldsymbol{b}' \boldsymbol{x} + \frac{1}{2} \boldsymbol{x}' \boldsymbol{H} \boldsymbol{x} = \Psi(\hat{\boldsymbol{x}}) + \nabla \Psi(\hat{\boldsymbol{x}}) \left(\boldsymbol{x} - \hat{\boldsymbol{x}}\right) + \frac{1}{2} (\boldsymbol{x} - \hat{\boldsymbol{x}})' \boldsymbol{H} \left(\boldsymbol{x} - \hat{\boldsymbol{x}}\right),$$

where $\boldsymbol{H} \triangleq \nabla^2 \Psi(\boldsymbol{x})$ is the Hessian of the cost function Ψ and the elements of \boldsymbol{H} are given by $H_{jk} = \frac{\partial^2}{\partial x_j \partial x_k} \Psi(\boldsymbol{x})$. (For a quadratic cost function this Hessian is independent of \boldsymbol{x} .) Recalling that $\Psi \Psi(\hat{\boldsymbol{x}}) = \boldsymbol{0}$ in the absence of constraints, we have

$$abla \Psi(\boldsymbol{x}^{(n)}) = \boldsymbol{H} \left(\boldsymbol{x}^{(n)} - \hat{\boldsymbol{x}} \right).$$

¹⁸Throughout this book, all superscripts (such as (n) and (n + 1)) on vectors such as \boldsymbol{x} denote iteration indices.

Subtracting \hat{x} from both sides of (1.11.1) and substituting in the above yields

$$\boldsymbol{x}^{(n+1)} - \hat{\boldsymbol{x}} = \boldsymbol{x}^{(n)} - \hat{\boldsymbol{x}} - \alpha_n \boldsymbol{D} \boldsymbol{H} \left(\boldsymbol{x}^{(n)} - \hat{\boldsymbol{x}} \right) = (\boldsymbol{I} - \alpha_n \boldsymbol{D} \boldsymbol{H}) (\boldsymbol{x}^{(n)} - \hat{\boldsymbol{x}}).$$
(1.11.2)

So the distance $x^{(n)} - \hat{x}$ to the solution should decrease each iteration if the matrix $I - \alpha_n DH$ is "small" in some appropriate sense.

For further insight, consider the penalized least-squares cost function (1.8.8) and suppose that A and R are circulant, D = I, and $K_{\varepsilon} = \sigma^2 I$. Then the Hessian is

$$oldsymbol{H} = rac{1}{\sigma^2}oldsymbol{A}'oldsymbol{A} + eta oldsymbol{\mathsf{R}} = Q^{-1}\left[rac{1}{\sigma^2}oldsymbol{\Gamma}'oldsymbol{\Gamma} + eta oldsymbol{\mathsf{\Pi}}
ight]Q,$$

where Q is a DFT matrix and Γ and Π were defined in §1.8.3. Let $E^{(n)} \triangleq Q(x^{(n)} - \hat{x})$ denote the DFT coefficients of the error vector at the *n*th iteration. Then from the recursion (1.11.2) we have

$$\boldsymbol{E}^{(n+1)} = \left(\boldsymbol{I} - \alpha_n \left(\frac{1}{\sigma^2} \boldsymbol{\Gamma}' \boldsymbol{\Gamma} + \beta \boldsymbol{\Pi}\right)\right) \boldsymbol{E}^{(n)}.$$

Therefore, all error frequency components will decrease at the *n*th iteration if and only if one chooses α_n such that

$$\left|1 - \alpha_n \left(\frac{\left|B_k\right|^2}{\sigma^2} + \beta \mathsf{R}_k\right)\right| < 1, \qquad \forall k$$

Of course, in the circulant case with a quadratic cost function, there is no need to use an iterative algorithm in the first place because a direct solution of the form (1.8.15) is available. But even in nonquadratic, non-circulant problems, similar convergence conditions arise, as discussed in more detail in Chapters 11 and 16.

1s, alg **1.11.2** Huber's iteration (s,res,npls,alg)

The recursive form of the "solution" (1.10.16) is suggestive of the following fixed-point iteration:

$$\begin{aligned} \boldsymbol{x}^{(n+1)} &= \left[\boldsymbol{A}' \boldsymbol{A} + \beta \boldsymbol{C}' \, \boldsymbol{D}(\boldsymbol{x}^{(n)}) \, \boldsymbol{C} \right]^{-1} \, \boldsymbol{A}' \boldsymbol{y} \\ &= \boldsymbol{x}^{(n)} - \left[\boldsymbol{A}' \boldsymbol{A} + \beta \boldsymbol{C}' \, \boldsymbol{D}(\boldsymbol{x}^{(n)}) \, \boldsymbol{C} \right]^{-1} \left(\left[\boldsymbol{A}' \boldsymbol{A} + \beta \boldsymbol{C}' \, \boldsymbol{D}(\boldsymbol{x}^{(n)}) \, \boldsymbol{C} \right] \boldsymbol{x}^{(n)} - \boldsymbol{A}' \boldsymbol{y} \right) \\ &= \boldsymbol{x}^{(n)} - \left[\boldsymbol{A}' \boldsymbol{A} + \beta \boldsymbol{C}' \, \boldsymbol{D}(\boldsymbol{x}^{(n)}) \, \boldsymbol{C} \right]^{-1} \, \nabla \Psi(\boldsymbol{x}^{(n)}), \end{aligned}$$
(1.11.3)

using (1.10.15). This is a form of **preconditioned gradient descent**. Often fixed-point iterations do not converge, but this algorithm, derived by Huber [90, p. 182], decreases $\Psi(x)$ monotonically each iteration, and converges to the minimizer of $\Psi(x)$ under mild conditions; see §14.5.4.4 and Chapter 15.

However, this algorithm is somewhat impractical for imaging problems due to the matrix inverse. Chapter 14 describes several practical alternatives. A particularly simple choice is the diagonally-preconditioned gradient descent method (14.6.13), which has the form

$$\boldsymbol{x}^{(n+1)} = \boldsymbol{x}^{(n)} - \mathsf{Diag}\left\{\frac{1}{d_{j}^{(n)}}\right\} \nabla \Psi(\boldsymbol{x}^{(n)})$$
(1.11.4)

$$d_{j}^{(n)} = \sum_{i=1}^{n_{\rm d}} |a_{ij}| |a|_{i} + \beta \sum_{k=1}^{K} |c_{kj}| |c|_{k} \omega_{\psi}([C\boldsymbol{x}^{(n)}]_{k}), \qquad (1.11.5)^{\text{e, res, npls, alg, def}}$$

where

$$|a|_i \triangleq \sum_{j=1}^{n_p} |a_{ij}|, \qquad |c|_k \triangleq \sum_{j=1}^{n_p} |c_{kj}|.$$

This iteration was used for the following example and for Fig. 1.11.1.

e, res, alg, xn-xh

s, res, ex1 1.11.3 Restoration example (s, res, ex1)

Fig. 1.11.1 illustrates the methods summarized in this chapter. The normalized root mean-squared (NRMS) errors of each method are shown along the vertical axis of each image, where

$$\text{NRMS} \triangleq \frac{\sqrt{\sum_{j=1}^{n_{\text{p}}} \left| \hat{x}_j - x_j \right|^2}}{\sqrt{\sum_{j=1}^{n_{\text{p}}} \left| x_j \right|^2}}$$

This figure of merit leaves much to be desired as a measure of image quality, but it serves as a starting point. Later chapters discuss more interesting figures of merit such as resolution (Chapter 24), noise (Chapter 25), and signal detection (Chapter 23).



Figure 1.11.1: Illustration of 2D image restoration by: unregularized methods, quadratically regularized least-squares methods, and edge-preserving nonquadratically regularized least-squares methods. Each vertical axis shows the corresponding NRMS error.

The figure includes the following images.

- The true object x_{true} , a grayscale image of the Greek word $\tau \delta \mu o \sigma$ ("a slice", the root of **tomography**) where white=100 and black=0.
- Noiseless blurry image $\bar{y} = Ax$ where A corresponds to shift-invariant blur having the separable PSF b[m, n] = b[n] b[m], where $b[n] = \left[\frac{1}{9}, \frac{1}{9}, \frac{5}{9}, \frac{1}{9}, \frac{1}{9}\right]$.
- Noisy blurry image $y = Ax + \varepsilon$ where the noise is zero-mean additive white gaussian distributed with $\sigma = 10$.
- The ML (inverse filter) reconstruction \hat{x}_{ML} defined in (1.6.9), computed via a circulant deconvolution approximation, both from the noiseless data \bar{y} and the noisy data y. For noiseless data, the deconvolution method works fine, but even for this moderately noisy data there is excessive noise amplification.
- In this case the image is (nearly) binary, so we can improve on \hat{x}_{ML} by rounding each pixel value in \hat{x}_{ML} to 0 or 100, whichever is nearer. (This is the ML classifier ignoring pixel correlations introduced by the deconvolution.) However, this only reduces the NRMS error from 141% to 114%.
- A quadratically penalized least-squares estimator computed using the first-order roughness penalty (1.10.1) in the penalized-likelihood cost function (1.8.1) which reduces to (1.8.8) because the noise is gaussian. The quadratic regularization reduces noise relative to y, but the edges are so seriously blurred that the overall NRMS error, which accounts for both noise and resolution effects, actually increases relative to y.

• Finally, a nonquadratically penalized least-squares estimate with hyperbola potential function and a 2nd-order neighborhood (including nearest diagonal neighbors), for $\delta = 0.1$ and $\beta = 2^8$. This approach gives the lowest NRMS of all methods shown for the noisy data. This example is ideal for such edge-preserving regularization because the true object is piece-wise smooth, indeed it is piece-wise constant.

Fig. 1.11.2 shows the weighting terms $\omega_{\psi}([C \hat{x}]_k)$ for the nonquadratic restoration example shown in Fig. 1.11.1. The weights are greatly reduced towards zero (black) from unity (white) near object edges, thereby helping preserve the edges in the restored image \hat{x} .

MIRT See restore_example.m.



Figure 1.11.2: Weighting terms $\omega_{\psi}([C \hat{x}]_k)$ associated with Fig. 1.11.1.

[RQ7]

fig tomos wpot

1.12 Sparsity models (s,res,sparse)

This section provides a brief overview of regulized image formation methods based on **sparsity** models. We discuss both **synthesis** and **analysis** formulations, also known as **generative models** and **discriminative models**.

1.12.1 Synthesis formulations (generative models)

In some applications the image itself is expected to be **sparse**, *e.g.*, when imaging some star fields [100] or in angiography [101]. In other applications, one might be willing to assume that the object is **sparse** with respect to some basis B. In such applications, we can "synthesize" the unknown image x in terms of a small number of basis vectors by writing

$$\boldsymbol{x} = \boldsymbol{B}\boldsymbol{z},\tag{1.12.1}$$

where B denotes a $n_p \times K$ matrix whose columns are basis vectors and z is an unknown vector of coefficients. In some cases B is overcomplete, meaning $K > n_p$. (In those cases, B is no longer a basis and often one uses generalizations called frames [102].) Sometimes B is selected to be a standard basis such as wavelets or the discrete cosine transform (DCT). In other cases, one learns B from the data [103–106]. In methods based on sparsity models, one expects only a small subset of the elements of z to be nonzero. Let $||z||_0$ denote¹⁹ the number of nonzero elements of z, *i.e.*,

$$\|\boldsymbol{z}\|_{0} \triangleq \sum_{k=1}^{K} \mathbb{I}_{\{\boldsymbol{z}_{k} \neq 0\}}.$$
(1.12.2)

Substituting the synthesis model (1.12.1) into the standard linear measurement model (1.4.4) yields the model

$$y = A \underbrace{Bz}_{x} + \varepsilon. \tag{1.12.3}$$

For such models, reasonable approaches to image recovery include the following.

¹⁹This norm notation is a slight abuse, because $\|\boldsymbol{x}\|_p \triangleq \left(\sum_j |x_j|^p\right)^{1/p}$ is a norm when $p \ge 1$ but not when p < 1. Nevertheless, when p < 1 the summation is still well defined, and one can show that $\|\boldsymbol{x}\|_p^p$ converges to $\|\boldsymbol{x}\|_0$ as $p \to 0$. Technically (1.12.2) is called **counting measure**, not a norm.

• Finding the image that best fits the data subject to a sparsity constraint:

$$\hat{\boldsymbol{ heta}} = \operatorname*{arg\,min}_{\boldsymbol{z}} \| \boldsymbol{y} - \boldsymbol{A}\boldsymbol{B}\boldsymbol{z} \| \, \, ext{s.t.} \, \, \| \boldsymbol{z} \|_{0} \leq L \in \mathbb{N},$$

where L < K. An iterative hard thresholding algorithm for this problem is derived in [107] using the optimization transfer methods of Chapter 14. The sparsity L is rarely known, so L is essentially a tuning parameter.

• Finding the sparsest set of coefficients for which the corresponding image fits the data exactly [101, 108]:

$$\hat{oldsymbol{ heta}} = rgmin_{oldsymbol{z}} \|oldsymbol{z}\|_0 \, \, ext{s.t.} \, oldsymbol{y} = oldsymbol{A}oldsymbol{B}oldsymbol{z}$$

This formulation is free of tuning parameters, but presumably is most useful only in the unlikely situation that the data is noiseless!

• Finding the sparsest set of coefficients for which the corresponding image fits the data to within some constraint:

$$\hat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{z}} \|\boldsymbol{z}\|_{0} \text{ s.t. } \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{B}\boldsymbol{z}\| \le \varepsilon.$$
(1.12.4)

This formulation may be particularly well suited to highly under-determined problems [109].

• Finding the image that minimizes a cost function that includes a data fidelity term and sparsity regularizer:

$$\hat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{z}} \frac{1}{2} \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{B}\boldsymbol{z}\|^2 + \beta \|\boldsymbol{z}\|_0. \qquad (1.12.5)$$

Often this regularized approach is equivalent, for suitable β and ϵ . to the constrained approach (1.12.4), but not always (particularly in nonconvex problems [110, 111]). The units of ϵ are more intuitive than those of β so (1.12.4) may simplify parameter selection. (See §2.5.2.1.) However, (1.12.4) is a constrained optimization problem so it may be more challenging to implement than (1.12.5).

• Including both a sparsity regularizer and another image regularizer:

$$\hat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{z}} \frac{1}{2} \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{B}\boldsymbol{z}\|^2 + \beta_1 \|\boldsymbol{z}\|_0 + \beta_2 \mathsf{R}(\boldsymbol{B}\boldsymbol{z}). \qquad (1.12.6)^{\text{e}, \text{ res, sparse, synth}}$$

All of the above estimates are in the synthesis form because after finding the estimate $\hat{\theta}$ of the coefficients we use (1.12.1) to synthesize the final image by computing $\hat{x} = B\hat{\theta}$.

1.12.2 Synthesis formulations: regularized

An equivalent way to write the regularized form (1.12.5) is:

$$\hat{\boldsymbol{x}} = \underset{\boldsymbol{x}}{\operatorname{arg\,min\,min}} \left\{ \frac{1}{2} \left\| \boldsymbol{y} - \boldsymbol{A} \boldsymbol{x} \right\|^2 + \beta \left\| \boldsymbol{z} \right\|_0 \right\} \text{ s.t. } \boldsymbol{x} = \boldsymbol{B} \boldsymbol{z}.$$
(1.12.7)

Note the strict equality constraint that corresponds to the model (1.12.1). Indeed, all of the formulations in §1.12.1 treat (1.12.1) as a strict constraint. However, the synthesis model (1.12.1) with sparse coefficient vector z may not be able to describe all signals of interest depending on the basis B and the sparsity of z.

An alternative to (1.12.7) is treat (1.12.1) as an *approximation*, *i.e.*, $x \approx Bz$ for some sparse z, suggesting that we use a regularizer rather than a constraint. One regularized version of (1.12.7) is:

$$\hat{\boldsymbol{x}} = \arg\min_{\boldsymbol{x}} \min_{\boldsymbol{z}} \left\{ \frac{1}{2} \| \boldsymbol{y} - \boldsymbol{A} \boldsymbol{x} \|_{2}^{2} + \beta_{1} \frac{1}{2} \| \boldsymbol{x} - \boldsymbol{B} \boldsymbol{z} \|_{2}^{2} + \beta_{2} \| \boldsymbol{z} \|_{0} \right\}.$$
(1.12.8)

An equivalent expression that more clearly reveals the regularizer is the following:

$$\hat{\boldsymbol{x}} = \operatorname*{arg\,min}_{\boldsymbol{x}} \left\{ \frac{1}{2} \left\| \boldsymbol{y} - \boldsymbol{A} \boldsymbol{x} \right\|_{2}^{2} + \beta_{1} \operatorname{\mathsf{R}}(\boldsymbol{x}) \right\}, \quad \operatorname{\mathsf{R}}(\boldsymbol{x}) \triangleq \operatorname{min}_{\boldsymbol{z}} \left\{ \frac{1}{2} \left\| \boldsymbol{x} - \boldsymbol{B} \boldsymbol{z} \right\|_{2}^{2} + \frac{\beta_{2}}{\beta_{1}} \left\| \boldsymbol{z} \right\|_{0} \right\}. \quad (1.12.9)$$

Here we see that R(x) favors images x that closely match Bz for some sparse coefficient vector z. These regularized forms are may be less sensitive to imperfections in the synthesis model, but have the drawback of requiring more tuning parameters.

1.12.3 Analysis formulations (discriminative models)

An alternative to the synthesis formulations above is to use an **analysis form** such as the following regularized cost function:

$$\hat{x} = \arg\min_{x} \frac{1}{2} \|y - Ax\|^{2} + \beta_{1} \|Cx\|_{0} + \beta_{2} \mathsf{R}(x), \qquad (1.12.10)^{\text{e, res, sparse}}$$

where here the rows of C are used to "analyze" the image x. The 0-norm penalizes the number of nonzero coefficients in the transform domain Cx. One can also define analysis formulations of the other variations in §1.12.1.

When C is **invertible**, the analysis form (1.12.10) is equivalent to the synthesis form (1.12.6) with $B = C^{-1}$ [112]. But more generally the analysis and synthesis forms differ and it is unclear which approach is best [112–114].

If C corresponds to the undecimated Haar analysis wavelets at the finest scale, which (in 1D) use the filter $\delta[n] - \delta[n-1]$, then this latter form is closely related to the roughness regularizer (1.8.3).

1.12.4 Convex relaxations

All of the above approaches have been investigated for imaging problems. The "norm" $||z||_0$ is nonconvex and nondifferentiable, greatly complicating minimization. Often it is replaced by $||z||_1$, which is convex. This replacement is called a **convex relaxation**. For example, often we replace the ℓ_0 regularized minimization problem (1.12.5) with:

$$\hat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{z}} \frac{1}{2} \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{B}\boldsymbol{z}\|^2 + \beta \|\boldsymbol{z}\|_1.$$
(1.12.11)

This problem is known as **least absolute shrinkage and selection operator** (LASSO) in the statistics literature [115–120]. This cost function also is non-differentiable at the origin, so conventional optimization algorithms for it can be quite slow. This is a very active research area with a rapidly growing literature. See [121–130].

When *A* is under-determined, yet another approach is **bi-level** optimization of the form [131]:

$$\underset{\boldsymbol{x}\in\mathcal{X}}{\arg\min}\,\mathsf{R}(\boldsymbol{x}) \text{ where } \mathcal{X} \triangleq \left\{ \underset{\boldsymbol{x}}{\arg\min}\,\|\boldsymbol{y}-\boldsymbol{A}\boldsymbol{x}\| \right\},$$

i.e., \mathcal{X} denotes the set of minimizers of a data-fit term.

For other variations such as **convolutional dictionary models** see §10.4.8.

1.13 Other formulations

s, res, line 1.13.1 Bayesian line-site models (s, res, line)

A nonquadratic but **convex potential function** can only *partially* preserve edges because large disparities between neighboring pixels are still discouraged, just less vigorously than the quadratic penalty function would. To penalize edges even less, one could use a **non-convex potential function** such as a **broken-parabola** function:

$$\psi(z) = \begin{cases} |z|^2/2, & |z| < \delta\\ \delta^2/2, & |z| \ge \delta. \end{cases}$$
(1.13.1)

This potential function, illustrated in Fig. 1.10.4, assigns the same cost $(\delta^2/2)$ to *any* value of the difference between two neighboring pixels exceeding δ .

Such potential functions are non-convex, which complicates the problem of finding the minimizer of the cost function $\Psi(x)$. Nevertheless, for piece-wise constant images, impressive restoration results have been reported.

Such methods originated in the Bayesian image restoration literature, but can be described equally well in the language of penalized-likelihood estimation. For neighboring pixels j and k, let l_{jk} denote a "line site" variable that should indicate the presence of an object edge "between" the jth and kth pixel. Typically we would like to have $l_{jk} = 1$ if there is an object intensity edge between pixels j and k, and to have $l_{jk} = 0$ if pixels j and k are both within an object region having uniform values. Intermediate values of l_{jk} can also be used if desired. Of course in practice we do not know which pixels are in the same region and which pairs straddle object edges, so we must estimate the l_{jk} values along with the object x.

If we *did* know good l_{jk} values, then in the same spirit as (1.10.17) we would want to use a roughness penalty function of the following form to avoid smoothing across edges:

$$\mathsf{R}(\boldsymbol{x},\boldsymbol{l}) = \sum_{j=1}^{n_{\rm p}} \sum_{k \in \mathcal{N}_j} (1 - l_{jk}) \frac{1}{2} |x_j - x_k|^2, \qquad (1.13.2)$$

where N_j denotes (half of) the set of neighbors of the *j*th pixel, as defined in §1.10, and where $l = \{l_{jk}\}$.

This formulation increases the number of unknowns from the n_p elements of x to at least $(1 + 2)n_p$ unknowns if we use l_{jk} parameters corresponding to horizontal and vertical neighbors. To provide a useful solution, we must include some type of penalty function for the l_{jk} values as well, to discourage unlikely configurations of edges. Let U(l) denote this penalty function. Then the overall penalized-likelihood estimate for such an approach is given by:

$$(\hat{\boldsymbol{x}}, \boldsymbol{l}) = \underset{\boldsymbol{x}, \boldsymbol{l}}{\operatorname{arg\,min}} \Psi(\boldsymbol{x}, \boldsymbol{l})$$
$$\Psi(\boldsymbol{x}, \boldsymbol{l}) = -\log \mathsf{p}(\boldsymbol{y} \mid \boldsymbol{x}) + \beta_1 \mathsf{R}(\boldsymbol{x}, \boldsymbol{l}) + \beta_2 U(\boldsymbol{l}), \qquad (1.13.3)$$

where each l_{jk} is constrained to the interval [0, 1]. One can show that as $\beta_2 \rightarrow 0$, $\hat{l}_{jk} \rightarrow 1$, because $\hat{l}_{jk} = 1$ minimizes (1.13.2), and \hat{x} degenerates to the ML estimate. So a nonzero β_2 and an appropriate U(l) are essential for this approach.

The simplest approach is to choose U(l) to count the number of edge sites:

$$U(l) = \sum_{j,k} l_{jk}.$$
 (1.13.4)

This penalty function discourages the formation of "too many" edges, but is indifferent to the shape of region boundaries. This is called a **non-interacting** line-site model. One can show [132–135] that this non-interacting model simplifies to ordinary penalized-likelihood estimation with the broken-parabola (1.13.1) as the potential function (Problem 1.13). One can show that replacing $\frac{1}{2} |x_j - x_k|^2$ with $|x_j - x_k|$ in (1.13.2) for a non-interacting model simplifies to ordinary PL estimation with a truncated absolute difference potential function [136] of the form $\psi(z) = \min(|z|, \beta_2/\beta_1)$.

To somewhat encourage object boundary continuity, line-site interactions are needed in the design of U(l). Most papers *e.g.*, [137–140], have used small **cliques** that have an inherently local effect and thus only partially encourage boundary continuity. There are also similar variational formulations, *e.g.*, [141].

In the context of blurred image restoration, comparatively large line-site neighborhood sizes that match the size of the PSF of the imaging system have been proposed [142, 143]. (How to apply that principle in tomography problems is unclear because each tomographic measurement is influenced by long strips traversing the entire object.) None of these line-site models address *global* connectivity or continuity of object boundaries, and thus are inherently local.

One of the few previous methods to capture global properties is a region-based Bayesian prior that has been applied successfully in tomography [144, 145]. That method uses discrete region identifiers (motivated by image segmentation problems) and assigns costs that prohibit disconnected regions, encourage regularly shaped regions, and discourage having too many regions. (The number of regions need not be specified *a priori*.) Some of these costs involve the entire image and are therefore global. The Bayesian formalism permits the exploration of estimate uncertainty, but using discrete region labels is challenging for computing point estimates.

An alternative method to encourage global boundary regularity is to use level sets to model object boundaries [146–148]. Such approaches are boundary based rather than region based; boundaries are continuous-valued, so simple gradient-descent methods are available for computing point estimates (at local minima of the cost function).

This book focuses on penalized-likelihood problems of the form (1.8.1) rather than on the line-site form (1.13.3). Nevertheless, many of the concepts would also apply to line-site formulations. When restoring multiple images simultaneously with common boundaries, line-site methods may be useful [149]. See §2.8.

1.13.2 Maximum entropy restoration (s,res,maxent)

An alternative to maximum-likelihood and penalized-likelihood methods are the **maximum entropy** methods for image restoration [150–163]. These methods use a version of **entropy** to quantify image smoothness or irregularity. (A uniform image, when treated as a uniform distribution, has high entropy, whereas an image that is a single Kronecker impulse has zero entropy in this framework.) This approach has been applied in many application domains, including spectral estimation [164] and tomographic reconstruction, *e.g.*, [44, 165–169].

Some maximum entropy formulations ignore measurement noise, e.g., [170], as follows:

$$\hat{m{x}} = rgmax_{m{x} \succeq m{0}} - \sum_{j=1}^{n_{
m p}} x_j \log x_j$$
 such that $m{y} = m{A}m{x}$

Other formulations allow for some noise, e.g.,

$$\hat{\boldsymbol{x}} = \operatorname*{arg\,max}_{\boldsymbol{x} \succeq \boldsymbol{0}} - \sum_{j=1}^{n_{\mathrm{p}}} x_j \log x_j \text{ such that } \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}\|^2 \le L\sigma^2,$$

where L is a parameter that one must select. By the theory of constrained optimization [47, p. 188], this latter approach is equivalent to a form of penalized least-squares estimation:

$$\hat{\boldsymbol{x}} = \operatorname*{arg\,min}_{\boldsymbol{x} \succeq \boldsymbol{0}} \frac{1}{2} \| \boldsymbol{y} - \boldsymbol{A} \boldsymbol{x} \|^2 + \beta \sum_{j=1}^{n_{\mathrm{p}}} x_j \log x_j,$$

for some value of β that depends on L above. In this setting, the (negative) entropy penalty function $\mathsf{R}(x) = \sum_{j=1}^{n_{\mathrm{p}}} x_j \log x_j$ is just one of many possible choices, as is not in any sense canonical. Yet another option (particularly for the under-determined case) is to choose, among all the LS solutions, the one having maximum entropy. Lyon et al. attempt this by minimizing $\mathsf{R}(x)$ subject to $x'\mathbf{1} = 1, x \succeq \mathbf{0}$, and $-A'(y - Ax) = \mathbf{0}$. The latter expression characterizes the family of *unconstrained* LS solutions, but not the set of nonnegativity-constrained LS solutions, so formulating maxent rigorously remains an open problem.

Although there are philosophical arguments that might be made in favor of maximum entropy in the absence of measurement noise, those arguments seem weaker in the presence of noise. The maximum entropy method is popular in astronomical image restoration because it favors "nearly black" objects [171, 172]. It is appropriately less popular in the tomographic imaging field.

s, res, super 1.13.3 Super-resolution problems (s, res, super)

This chapter has focused on restoring an image x from a single noisy, blurred image y. In some applications one can acquire *multiple* images y_1, \ldots, y_K each of which is related to a single unknown image x by a possibly different system model A_k and noise model:

$$\boldsymbol{y}_k = \boldsymbol{A}_k \boldsymbol{x} + \boldsymbol{\varepsilon}_k.$$

If the system models differ by subpixel spatial translations, then one can attempt to recover x at a finer spatial resolution than the measured images $\{y_k\}$. This problem is known as super-resolution. A typical approach is based on a cost function of the form (for white gaussian noise):

$$\Psi(oldsymbol{x}) = \sum_{k=1}^{K} rac{1}{2} \left\|oldsymbol{y}_k - oldsymbol{A}_k oldsymbol{x}
ight\|^2 + \mathsf{R}(oldsymbol{x}) \,.$$

In many cases, the system model A_k depends on motion parameters that one also must estimate. See references [173–190] and these surveys [191, 192]. For medical imaging applications, including some controversies, see [193–202].

1.14 Summary (s,res,summ)

This chapter has used the image restoration application as a vehicle for introducing many of the concepts and notational conventions that are used throughout this *book* for image reconstruction problems. The principal concepts include

- the deficiencies of inverse filtering (deconvolution),
- matrix-vector representation of linear models for imaging systems,
- circulant approximations for linear shift-invariant problems,
- ML, MAP, and penalized-likelihood estimation criteria,
- and roughness penalty functions and their effects.

The field of image restoration remains an active area of research with a growing number of applications.

1.15 **Problems** (s,res,prob)

Problem 1.1 An image restoration method uses object model (1.3.6) with a 2D rectangular basis function: $\beta_0(x,y) =$ $\operatorname{rect}_2(x/\triangle_x, y/\triangle_y)$. The sensor is shift invariant with a rectangular blur: $b(x,y) = \frac{1}{4\triangle_x \triangle_y} \operatorname{rect}_2\left(\frac{x}{2\triangle_x}, \frac{y}{2\triangle_y}\right)$. Assuming zero end conditions, determine the values of elements a_{ij} of the system matrix A. Assume both the spacing of the sensor elements and the spacing of the object basis functions are $(\triangle_x, \triangle_y)$.

Problem 1.2 Consider a 1D signal restoration problem for a linear shift-invariant system with additive white gaussian noise and impulse response

 $b[n] = \delta[n-2] + 8\,\delta[n] + \delta[n+2]\,.$

Would the deconvolution method be a suitable restoration approach for this system? Explain why or why not.

Problem 1.3 Derive the circular convolution formulas (1.4.11) and (1.4.12) for periodic boundary conditions.

Problem 1.4 Use the principles of §1.4.3.1 to find analytically the eigenvalues and eigenvectors of the following matrix

$$\begin{bmatrix} 5 & 2 & 1 & 0 & 1 & 2 \\ 2 & 5 & 2 & 1 & 0 & 1 \\ 1 & 2 & 5 & 2 & 1 & 0 \\ 0 & 1 & 2 & 5 & 2 & 1 \\ 1 & 0 & 1 & 2 & 5 & 2 \\ 2 & 1 & 0 & 1 & 2 & 5 \end{bmatrix}$$

Verify your eigenvalues using MATLAB's eig function. Your eigenvectors may differ from those of MATLAB; why?

Problem 1.5 Consider a 1D system with impulse response $b[n] = 3\delta[n] + \delta[n-1] + \delta[n+1]$. Using MATLAB's eig command, compute and plot the "exact" eigenvalues of the Toeplitz representation (1.4.7) for N = 8, N = 16, and N = 128. Determine analytically the eigenvalues of the circulant approximation (1.4.13) for N = 1000 and superimpose on the preceding plot. For superposition, sort the eigenvalues from largest to smallest, and normalize the eigenvalue indices as (k-1)/N. Discuss.

s,res,prob

Problem 1.6 [204, Eqn. (2.7)] states that $\lambda_{\min}(A) \leq \lambda_{\min}(c(A)) \leq \lambda_{\max}(c(A)) \leq \lambda_{\max}(A)$, where c(A) is a certain circulant approximation to A. These inequalities provide the following bound on the condition number (28.7.2):

$$\kappa(\mathbf{A}'\mathbf{A}) = \frac{\lambda_{\max}(\mathbf{A}'\mathbf{A})}{\lambda_{\min}(\mathbf{A}'\mathbf{A})} \ge \frac{\lambda_{\max}(c(\mathbf{A}'\mathbf{A}))}{\lambda_{\min}(c(\mathbf{A}'\mathbf{A}))} = \kappa(c(\mathbf{A}'\mathbf{A})).$$
(1.15.1)

Evaluate these bounds for the preceding problem and compare to the eigenvalues of the Toeplitz matrices. See also [205, 206]. (Need typed.)

Problem 1.7 Can you find bounds that are the other way around? Possible resources: [204, 207–210] and citations therein. (Solve?)

Problem 1.8 Determine A for the mirror end conditions discussed in §1.4. (Need typed.)

Problem 1.9 Generalize the expression (1.4.20) or (1.4.21) to the case of replicated end conditions. (Solve?)

Problem 1.10 If a matrix M is square and circulant, then computing QMQ^{-1} will yield an exactly diagonal matrix, where Q is the DFT matrix defined in (1.4.29). Consider the following four representations of a system matrix A: (1.4.7), (1.4.9), (1.4.10), and (1.4.13). For each representation, using MATLAB to compute $D = QA'AQ^{-1}$ for the impulse response $b[n] = \delta[n-1] + 2\delta[n] + \delta[n+1]$ and for N = 64. (Hint: you can create each of the A matrices needed in one or two lines of MATLAB using convmtx.) Display for yourself the D matrices to visualize how close to diagonal they are. Compute the fractional off-diagonal "energy" as follows:

$$\frac{\sqrt{\sum_{k\neq j} |d_{kj}|^2}}{\sqrt{\sum_{k,j} |d_{kj}|^2}}.$$

Compare the four models using this quantitative measure of "non-circulant-ness."

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e,res,circ,cond

Problem 1.11 Consider the statistical model $y_i \sim \text{Poisson}\{a_ix\}$ where x is an unknown nonnegative scalar and $a_i = i^2$, i = 1, ..., 5. Find expressions for the log-likelihood and the ML estimate of x given $y_1, ..., y_5$.

Problem 1.12 For any $n_p \times n_p$ unitary matrix U, consider the regularized LS cost function

$$\Psi(\boldsymbol{z}) = rac{1}{2} \| \boldsymbol{y} - \boldsymbol{U} \boldsymbol{z} \|^2 + eta \sum_{j=1}^{n_{\mathrm{p}}} \psi(z_j) \,.$$

• Defining b = U'y, and using the fact that

$$\|m{y} - m{U}m{z}\|^2 = \|m{U}'m{y} - m{z}\|^2 = \|m{b} - m{z}\|^2 = \sum_{j=1}^{n_{\mathrm{p}}} |b_j - z_j|^2,$$

find an analytical solution for \hat{z} in terms of b, for the l_1 regularized case where $\psi(z) = |z|$. Sketch \hat{z}_i vs $b_i \in \mathbb{R}$.

- Compare (by plotting or sketching) to the solution when an l_2 penalty is used where $\psi(z) = \frac{1}{2} |z|^2$. Repeat for at least one more of the following potential functions.
- l_0 potential: $\psi(z) = \mathbb{I}_{\{z \neq 0\}}$.
- The truncated absolute value potential: $\psi(z) = \min(|z|, \delta)$.
- The broken parabola potential: $\psi(z) = \min\left(\frac{1}{2}|z|^2, \frac{1}{2}\delta^2\right)$.
- Huber potential (1.10.9).
- Generalized-gaussian potential (challenging!): $\psi(z) = |z|^p$, for $p \neq 1$. (Focus on $p \in \{1/2, 4/3, 3/2, 2, 3, 4\}$ [211].) For other values of p, see Newton's method in [212].
- The hyperbola potential (challenging!): $\psi(z) = \delta^2(\sqrt{1 + |z/\delta|^2 1})$. This problem relates to wavelet-based **denoising** using shrinkage [213] and soft thresholding [214, 215].

Problem 1.13 Show that when the non-interacting line-site penalty function (1.13.4) is used in the joint penalizedlikelihood estimator (1.13.3), the solution to \hat{x} reduces to the ordinary penalized-likelihood form (1.8.1) with R(x) as in (1.10.10) and ψ as the **broken parabola** in (1.13.1).

Problem 1.14 Let D_N denote the $(N-1) \times N$ one-dimensional finite-differencing matrix shown in (1.8.4), and I_N denote the $N \times N$ identity matrix. Show that the simple quadratic penalty (1.10.1) that uses only horizontal and vertical differences can be written in the form (1.10.7), where C is the following $[N(M-1) + M(N-1)] \times MN$ matrix:

$$\boldsymbol{C} = \begin{bmatrix} \boldsymbol{I}_N \otimes \boldsymbol{D}_M \\ \boldsymbol{D}_N \otimes \boldsymbol{I}_M \end{bmatrix}, \qquad (1.15.2)$$

and " \otimes " denotes the *Kronecker product* defined in (28.1.12).

Problem 1.15 For regularized restoration of a $M \times N$ image using a penalty function $\mathsf{R}(\boldsymbol{x}) = \frac{1}{2} \|\boldsymbol{C}\boldsymbol{x}\|^2$, one option is to use

$$\boldsymbol{C} = \begin{bmatrix} \boldsymbol{D}_{MN} \\ \boldsymbol{T} \end{bmatrix}, \tag{1.15.3}$$

where T is an $M(N-1) \times MN$ Toeplitz matrix with first row $[-1 \mathbf{0}'_{M-1} \mathbf{1} \mathbf{0}'_{MN-M-1}]$, where $\mathbf{0}'_K$ denotes the row vector of K zeros. Another option is to use C defined in (1.15.2). Using (1.15.3) may be slightly faster (in ANSI C). Explain the advantage of using (1.15.2).

Problem 1.16 The 1D regularizer Hessian matrix in (1.8.6) has eigenvalues given in footnote 13. Consider the 2D regularizer C for a $M \times N$ image given in (1.15.2), and define the Hessian matrix $\mathbf{R} = C'C$. Determine analytically the eigenvalues of R.

Problem 1.17 Consider the discrete-space denoising problem with no boundary conditions and zero-mean white noise:

$$g[n] = f[n] + \varepsilon[n], \quad n \in \mathbb{Z},$$

Analyze the spatial resolution properties of the following quadratically-regularized denoising estimator for $\beta > 0$:

$$\hat{f} = \operatorname*{arg\,min}_{f \in \ell_2} \sum_{n = -\infty}^{\infty} \frac{1}{2} |g[n] - f[n]|^2 + \beta \sum_{n = -\infty}^{\infty} \frac{1}{2} |f[n] - f[n-1]|^2.$$

e,res,C,kror

Hint. Using the DTFT, first find the frequency-domain relationship between $\mathsf{E} \left| \hat{f} \right|$ *and f.*

Optional: show that $\mathsf{E}[\hat{f}] = h * f$, *where the impulse response is*

$$h[n] = ab^{|n|} = a e^{-|\log b||n|}, \quad b = \frac{1 + 2\beta - \sqrt{1 + 4\beta}}{2\beta} = \frac{2\beta}{1 + 2\beta + \sqrt{1 + 4\beta}}$$

where $a = \frac{1+b^2}{1-b^2}\frac{1}{1+2\beta}$. Note that 0 < b < 1. Use §29.6.1. This is one of the few cases where we can find an explicit expression for the impulse response of a regularized problem [216, 217]. Determine the FWHM of the impulse response in terms of b.

Problem 1.18 Generalize Problem 1.17 to the case where the regularizer is $\sum_{n=-\infty}^{\infty} \frac{1}{2} |c[n] * f[n]|^2$, where the filter c[n] corresponds to **2nd-order finite differences**: $c[n] = 2\delta[n] - \delta[n-1] - \delta[n+1]$. This is called **Hodrick-Prescott** filtering [218] in some fields.

Problem 1.19 Generalize Problem 1.17 to the case where the regularizer is $\sum_{n=-\infty}^{\infty} \frac{1}{2} |f[n] - c[n] * f[n]|^2$, where the filter h[n] is the 3-point moving average: $c[n] = \frac{1}{3} (\delta[n] + \delta[n-1] + \delta[n+1])$.

Problem 1.20 Consider the 3D discrete-space denoising problem with no boundary conditions and zero-mean white noise:

$$g[l,m,n] = f[l,m,n] + \varepsilon[l,m,n], \quad l,m,n \in \mathbb{Z},$$

Analyze the spatial resolution properties of the following quadratically-regularized denoising estimator for $\beta_i > 0$:

$$\begin{split} \hat{f} &= \operatorname*{arg\,min}_{f \in \ell_2(\mathbb{Z}^3)} \sum_{l,m,n=-\infty}^{\infty} \frac{1}{2} \left| g[l,m,n] - f[l,m,n] \right|^2 + \beta_1 \sum_{l,m,n=-\infty}^{\infty} \frac{1}{2} \left| f[l,m,n] - f[l-1,m,n] \right|^2 \\ &+ \beta_2 \sum_{l,m,n=-\infty}^{\infty} \frac{1}{2} \left| f[l,m,n] - f[l,m-1,n] \right|^2 \\ &+ \beta_3 \sum_{l,m,n=-\infty}^{\infty} \frac{1}{2} \left| f[l,m,n] - f[l,m,n-1] \right|^2. \end{split}$$

Optional: Think about the case of anisotropic 3D voxel and how one would adjust $\{\beta_i\}$ *to get reasonably similar FWHM in all three directions.* (Solve?)

Problem 1.21 Analyze the spatial resolution properties of the following different denoising problems, where in each case we form an estimate $\hat{f} = \arg \min_{f} \Psi(f)$.

• Continuous-continuous formulation (use Fourier transform):

$$\Psi(f) = \frac{1}{2} \|g - f\|^2 + \beta \int \frac{1}{2} |\dot{f}|^2$$

• Continuous-discrete formulation (use Fourier series?):

$$\Psi(f) = \sum_{n=0}^{N-1} \frac{1}{2} |g_n - f(n/N)|^2 + \beta \int_0^1 \frac{1}{2} \left| \dot{f} \right|^2.$$

In each case one can find an expression similar to (1.9.1) *or* (1.9.2). *Hint. Yet another formulation is the finite-length discrete case with periodic end conditions:*

$$\Psi(f) = \sum_{n=0}^{N-1} \frac{1}{2} |g[n] - f[n]|^2 + \beta \sum_{n=0}^{N-1} \frac{1}{2} |f[n] - f[n \mod N]|^2$$

Letting F_k denote the N-point DFT of f[n], by **Parseval's relation** for the DFT, we can express the cost function as

$$\sum_{n=0}^{N-1} \frac{1}{2} \left| G_k - F_k \right|^2 + \beta \sum_{n=0}^{N-1} \frac{1}{2} \left| F_k - e^{-i2\pi k/N} F_k \right|^2 = \sum_{n=0}^{N-1} \frac{1}{2} \left| G_k - F_k \right|^2 + \beta \sum_{n=0}^{N-1} \mathsf{R}_k \frac{1}{2} \left| F_k \right|^2$$

where $R_k = |1 - e^{-i2\pi k/N}|^2 = 2 - 2\cos(2\pi k/N)$. Differentiating w.r.t. F_k and equating to zero yields $\hat{F}_k = L_k G_k$, where L_k was defined in (1.8.16), so the resolution properties here are $E[\hat{F}_k] = \frac{1}{1+\beta R_k}F_k$.

n ras orn difts

,res,srp,dtft,ma

p,res,srp

Problem 1.22 Consider the 1D continuous-space denoising problem $g(t) = f(t) + \varepsilon(t)$ with estimator

$$\hat{f} = \operatorname*{arg\,min}_{f} \Psi(f), \qquad \Psi(f) = \int \frac{1}{2} |g(t) - f(t)|^2 \, \mathrm{d}t + \beta \int \frac{1}{2} \left| f^{(p)}(t) \right|^2 \, \mathrm{d}t,$$

where $f^{(p)}$ denotes the pth derivative of f. Analyze the spatial resolution properties of the estimator \hat{f} . (i) Find a general expression for the frequency response, akin to (1.9.2). (ii) Using [220] and/or §29.4.1, verify the following specific expressions for the impulse response for p = 1 (1st-order regularization) and p = 2 (2nd-order regularization):

$$h_1(t) = \frac{1}{2\sqrt{\beta}} e^{-|t|/\sqrt{\beta}}, \qquad h_2(t) = \frac{1}{2\beta^{1/4}} e^{-|t|/(\sqrt{2}\beta^{1/4})} \sin\left(\frac{|t|}{\sqrt{2}\beta^{1/4}} + \frac{\pi}{4}\right).$$

(iii) Show also that $FWHM_1 = (2 \log_2)\beta^{1/2}$ and $FWHM_2 \propto \beta^{1/4}$. (iv) Use the plot in Fig. 1.15.1 of these two PSFs (at matched FWHM) to compare them qualitatively. (v) For even $p \ge 2$ and $\beta = 1$, use §29.4.1 to find a general expression for the impulse response of the following form:

$$h_p(t) = \frac{1}{p} \sum_{l=0}^{p/2-1} \left[\frac{b_l^2}{a_l} \cos(b_l t) + \frac{a_l^2}{b_l} \sin(b_l |t|) \right] e^{-a_l |t|} .$$
(1.15.4)



Figure 1.15.1: PSFs of 1st-order and 2nd-order regularization for 1D continuous-space denoising.

p,res,up2

Problem 1.23 Consider the 1D "regularized interpolation" or "super-resolution" problem, where we measure the even (or odd) samples of a 1D signal x[n] with noise:

$$y[n] = x[2n] + \varepsilon[n],$$

and we wish to recover $x[\cdot]$ by a quadratically penalized LS method:

$$\hat{x} = \arg\min_{x} \sum_{n=-\infty}^{\infty} \frac{1}{2} |y[n] - x[2n]|^2 + \beta \sum_{n=-\infty}^{\infty} \frac{1}{2} |(c * x)[n]|^2,$$

where c[n] is a (typically high-pass) filter. We want to determine the frequency-domain relationship between $\hat{x}[n]$ and y[n]. Towards this end, consider the model $y_k[n] = s_k[n] + \varepsilon_k[n]$ where for k = 0, 1:

$$s_k[n] = \frac{1 + (-1)^k (-1)^n}{2} x[n] \stackrel{\text{DTFT}}{\longleftrightarrow} S_k(\Omega) = \frac{X(\Omega) + (-1)^k X(\Omega \pm \pi)}{2}.$$

So $y_0[n]$ is the even samples and $y_1[n]$ is the odd samples of x[n] plus noise. Let

$$\hat{x}_k = \underset{x}{\arg\min} \sum_{n} \left| y_k[n] - \frac{1 + (-1)^k (-1)^n}{2} x[n] \right|^2 + \beta \sum_{n} \left| (c * x)[n] \right|^2.$$

- Determine the frequency domain relationship between $\hat{x}_k[n]$ and $y_k[n]$.
- Does regularization overcome the possible aliasing associated with down sampling a signal?

Problem 1.24 Continuing Problem 1.23, analyze the resolution properties. Let $\hat{x} \triangleq \frac{1}{2} (\hat{x}_0 + \hat{x}_1)$, and show that $\mathsf{E}[\hat{X}(\Omega)] = L(\Omega)X(\Omega)$ where $L(\Omega) = \frac{R(\Omega \pm \pi)}{R(\Omega + R(\Omega \pm \pi) + 2\beta R(\Omega)R(\Omega \pm \pi))}$.

Problem 1.25 Generalizing Problem 1.23, consider a 1D "super-resolution" problem where we measure every 3rd sample of a blurred 1D signal x[n], n = 0, ..., N - 1 with noise:

$$y[m] = (b * x)[3m] + \varepsilon[m], \quad m = 0, \dots, M - 1,$$

where in this problem we consider periodic convolution throughout and N = 3M. Here we recover $x[\cdot]$ by a quadratically penalized LS method expressed in a matrix formulation:

$$\hat{x} = \operatorname*{arg\,min}_{m{x}} rac{1}{2} \|m{y} - m{A}m{x}\|_2^2 + rac{1}{2} \|m{C}m{x}\|_2^2$$

where C'C is a circulant matrix, typically representing a high-pass filter, and A = SB is a $M \times N$ matrix where B is a $N \times N$ circulant matrix corresponding to the blur b[n] and $S = I_N \otimes [1 \ 0 \ 0]$ is a $M \times N$ "down-sampling" matrix. Find a matrix expression for the solution and show how one can use FFT's to implement that solution efficiently. Note that A is not circulant (it is rectangular) nor is A'A is circulant.

Problem 1.26 This problem considers whether the penalized least-squares cost function $\Psi(\mathbf{x})$ in (1.10.11) has a *unique minimizer* in the usual cases where \mathbf{A} and \mathbf{C} have disjoint null spaces (other than $\mathbf{0}$).

- Prove that if the potential function ψ used in (1.10.11) is twice differentiable with a positive second derivative, then Ψ is strictly convex (and thus has a unique minimizer).
- What if ψ is strictly convex, but does not necessarily have a positive second derivative? An example would be $\psi(z) = |z|^4$.
- What if ψ is merely convex, like the Huber function? Hint: see Fig. 1.15.2.



Figure 1.15.2: Contours of data-fit term, regularizer, and cost function $\Psi(x)$ for Problem 1.26.

p,res,fixed

Problem 1.27 Consider the regularized least-squares problem (1.10.11) with regularizer (1.10.10) and the usual 1st-order finite differencing matrix C.

- Ken uses the generalized-gaussian potential function $\psi(z) = |z|^q$ with q = 1.5, and states that the solution \hat{x} satisfies the recursive expression (1.10.16). Discuss.
- Maria uses the Geman & McClure potential function $\psi(z) = |z|^2 / (1 + |z|^2)$ and also states that the solution \hat{x} satisfies the recursive expression (1.10.16). Discuss.

Problem 1.28 Use circulant end conditions to synthesize a gaussian random field image like that in Fig. 1.7.1, for the 2D finite differencing matrix C defined in (1.10.8).

Hint. The goal is to draw $\boldsymbol{x} \sim N(\boldsymbol{0}, \boldsymbol{K}_{\boldsymbol{x}})$, so let $\boldsymbol{x} = \boldsymbol{K}_{\boldsymbol{x}}^{1/2} \boldsymbol{w}$ where $\boldsymbol{w} \sim N(\boldsymbol{0}, \boldsymbol{I})$. In this case, $\boldsymbol{K}_{\boldsymbol{x}} = [\boldsymbol{C}'\boldsymbol{C}]^{-1}$. Because $\boldsymbol{K}_{\boldsymbol{x}}$ is not invertible, use its pseudoinverse. Do not use the pinv command; use FFTs.

fig prob res con

Problem 1.29 Any (stationary) gaussian random field (GRF) is defined solely by its mean and autocorrelation function. Fig. 1.15.3 illustrates that the autocorrelation of a random field provides limited insight into its nature. The random process y[m, n] was generated by filtering white noise with the filter $h_1[m, n] = \mathbb{I}_{\{|n| \le 2\}}\mathbb{I}_{\{|m| \le 2\}}$. Random process z[m, n] was generated by first defining a Bernoulli random field that takes the value 1 - p with probability p and the value -p with probability 1 - p for some $p \in (0, 1)$, and then convolving that field with the filter $h_2[m, n] = h_1[m, n] / \sqrt{p(1-p)}$. Show that y[m, n] and z[m, n] have identical mean and autocorrelation functions.



Figure 1.15.3: Two different wide-sense stationary random fields with identical mean and autocorrelation functions.

p,res,psf,noise

Problem 1.30 Consider a 1D deconvolution problem with blur $b[n] = \frac{1}{4} \delta[n+1] + \frac{1}{2} \delta[n] + \frac{1}{4} \delta[n-1]$. Assuming periodic end conditions for N = 64, use the circulant analyses of §1.8.3 and §1.9 to make a single plot showing the trade-off between spatial resolution (such as FWHM of the PSF) and noise (Var{ \hat{x}_j } / σ^2) over a range of values of β . (Horizontal axis should be FWHM; vertical axis should be noise standard deviation: $\sqrt{Var{\hat{x}_j}}$. Plot curves for regularization based on both first- and second-order finite differences and compare.

Problem 1.31 The *iterated conditional modes* (*ICM*) algorithm [221] for MAP estimation from the model $y = x + \varepsilon$ uses the following recursion:

$$x_j^{(n+1)} = \operatorname*{arg\,max}_{x_j} \mathsf{p}\Big(x_j \,|\, y_j, \boldsymbol{x}_{\mathcal{N}_j}^{(n)}\Big) = \operatorname*{arg\,max}_{x_j} \left[\log(\mathsf{p}(y_j \,|\, x_j)) + \log\Big(\mathsf{p}\Big(x_j \,|\, \boldsymbol{x}_{\mathcal{N}_j}^{(n)}\Big)\Big) \right],$$

where \mathcal{N}_j denotes the neighborhood of the *j*th pixel.

Derive the ICM algorithm for the case where ε is zero-mean white gaussian noise with variance σ^2 and where the MRF prior has (improper) gaussian distribution: $\mathbf{p}(\mathbf{x}) = \frac{1}{Z} e^{-\frac{\beta}{2} \mathbf{R}(\mathbf{x})}$ with $\mathbf{R}(\mathbf{x}) = \sum_{n=0}^{N-1} \frac{1}{2} |\mathbf{x}[n] - \mathbf{x}[(n-1) \mod N]|^2 = \frac{1}{2} ||\mathbf{C}\mathbf{x}||^2$ where \mathbf{C} is the circulant finite-differencing matrix defined in (1.8.12). Show that this ICM algorithm is convergent by relating it to a gradient descent (GD) algorithm with a suitable step size.

Problem 1.32 From §1.8.3, image denoising with quadratic regularizer (1.8.11) is equivalent to applying a low-pass Wiener-like filter (1.8.16) with frequency response

$$L_{\mathrm{IIR}}(\Omega) = rac{1}{1 + eta R(\Omega)}, \quad R(\Omega) = 2 - 2\cos(\Omega).$$

IIg_prob_res_autc

This is an **IIR filter** and in some situations it may be preferable to use a **FIR filter**. Rearranging, we can solve for $\beta R(\Omega)$ in terms of $L(\Omega)$ to design a IIR regularizer for a given desired response $L(\Omega)$:

$$\beta R(\Omega) = \frac{1}{L(\Omega)} - 1.$$

Because quadratic regularization blurs edges, often we would use a small value of β , so the FWHM of the low-pass filter is at most 2 or 3 pixels, in which case a FIR filter need only have a few taps, for which

$$L_{\rm FIR}(\Omega) = b_0 + 2b_1 \cos(\Omega) + 2b_2 \cos(2\Omega) \,.$$

Determine the values of the FIR filter taps b_0, b_1, b_2 so that $L_{\text{FIR}}(0) = L_{\text{IIR}}(0), L_{\text{FIR}}(\pi) = L_{\text{IIR}}(\pi), and \frac{d}{d\Omega} L_{\text{FIR}}(\Omega) \le 0, \ 0 \le \Omega \le \pi.$

Problem 1.33 Prove or disprove whether the following two sparsity formulations are equivalent if B is a Parseval tight frame

(restricted) synthesis: $\hat{x} = B\hat{\theta}$, $\hat{\theta} = \operatorname*{arg\,min}_{z} \|z\|_{p}$ sub. to $\|y - ABz\|_{2} < \varepsilon$ and B'Bz = z

analysis: $\hat{\boldsymbol{x}} = \operatorname*{arg\,min}_{\boldsymbol{x}} \|\boldsymbol{B}'\boldsymbol{x}\|_p$ sub. to $\|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}\|_2 < \varepsilon$.

(Solve?)

1.16 **Bibliography**

lagendijk:91

snyder:95:cfr

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