II. Linear Estimation using Least Squares

In this chapter of the course, we will focus on problems of the form:

$$\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}$$

$$(\text{vector in } \mathbb{R}^M) = (M \times N \text{ matrix})(\text{vector in } \mathbb{R}^N).$$

We are given $\boldsymbol{A}$, we observe $\boldsymbol{y}$ and want to find (or estimate) $\boldsymbol{x}$.

This is called a **linear inverse problem**, and is one of the most important and fundamental concepts in all of engineering, science, and applied mathematics.

We will start by looking at two areas of interest in which problems like this naturally arise.

Supervised Learning

The fundamental supervised learning problem is to estimate a function $f(\boldsymbol{t})$ on $\mathbb{R}^D$ from observations of its samples. Given pairs $(\boldsymbol{t}_m, y_m)$, $m = 1, \ldots, M$ with $\boldsymbol{t}_m \in \mathbb{R}^D$ and $y_m \in \mathbb{R}$, we want to find $f : \mathbb{R}^D \to \mathbb{R}$ such that

$$f(\boldsymbol{t}_m) \approx y_m, \quad m = 1, \ldots, M.$$

As stated, this is not a well-posed problem, as there are of course many functions that can match a set of samples at a finite number of points.

To make the problem well-posed, we need a clearly defined set of functions $\mathcal{F}$ from which to choose f. Choosing $\mathcal{F}$ is essentially a modeling problem, and there are many interesting ways in which it might be done. One way which we will examine thoroughly is to make $\mathcal{F}$ a *linear subspace* of mappings.

Example: Linear regression

One reasonable (and classical) model is for $\mathcal{F}$ to contain the set of all **linear functionals** on $\mathbb{R}^D$. A linear functions on $\mathbb{R}^D$ is a mapping $f : \mathbb{R}^D \rightarrow \mathbb{R}$ that obeys

$$f(\alpha \boldsymbol{t}_1 + \beta \boldsymbol{t}_2) = \alpha f(\boldsymbol{t}_1) + \beta f(\boldsymbol{t}_2),$$

for all $\alpha, \beta \in \mathbb{R}$ and $\boldsymbol{t}_1, \boldsymbol{t}_2 \in \mathbb{R}^D$. It is a fact[1] that every linear functional on $\mathbb{R}^D$ is uniquely represented by a vector $\boldsymbol{x}_f \in \mathbb{R}^D$, where

$$f(\boldsymbol{t}) = \langle \boldsymbol{t}, \boldsymbol{x}_f \rangle.$$

So given the $(\boldsymbol{t}_m, y_m)$, we want to find $\boldsymbol{x}$ such that

$$y_m = \langle \boldsymbol{t}_m, \boldsymbol{x} \rangle,$$

and in cases where it is not possible for equality to hold exactly above for all m, we want the "best" $\boldsymbol{x}$ possible.

Stacking up the $\boldsymbol{t}_m$ as rows in a $M \times D$ matrix $\boldsymbol{A}$ gives us

$$\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}, \quad \text{where} \quad \boldsymbol{A} = \begin{bmatrix} - & \boldsymbol{t}_1^{\mathrm{T}} & - \\ - & \boldsymbol{t}_2^{\mathrm{T}} & - \\ & \vdots & \\ - & \boldsymbol{t}_M^{\mathrm{T}} & - \end{bmatrix}, \quad \boldsymbol{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_M \end{bmatrix}.$$

Example: Nonlinear regression using a basis

Another reasonable model for $\mathcal{F}$ is that it is a (finite-dimensional) subspace spanned by basis functions $\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_N$. That is, we can

[1] The name by which this fact goes is the *Riesz Representation Theorem*, and it holds not just in $\mathbb{R}^D$, but in any Hilbert space (at least for linear functionals that are also continuous).

write

$$f(\boldsymbol{t}) = \sum_{n=1}^{N} x_n \psi_n(\boldsymbol{t}).$$

Again, fitting a function in this space $\mathcal{F}$ is the same as fitting a $\boldsymbol{x} \in \mathbb{R}^N$ such that

$$\begin{aligned} y_1 &= \sum_{n=1}^{N} x_n \psi_n(\boldsymbol{t}_1), \\ y_2 &= \sum_{n=1}^{N} x_n \psi_n(\boldsymbol{t}_2), \\ &\vdots \\ y_M &= \sum_{n=1}^{N} x_n \psi_n(\boldsymbol{t}_M). \end{aligned}$$

We can rewrite this as

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_M \end{bmatrix} = \begin{bmatrix} \psi_1(\boldsymbol{t}_1) & \psi_2(\boldsymbol{t}_1) & \cdots & \psi_N(\boldsymbol{t}_1) \\ \psi_1(\boldsymbol{t}_2) & \psi_2(\boldsymbol{t}_2) & \cdots & \psi_N(\boldsymbol{t}_2) \\ \vdots & & \ddots & \\ \psi_1(\boldsymbol{t}_M) & \psi_2(\boldsymbol{t}_M) & \cdots & \psi_N(\boldsymbol{t}_M) \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix},$$

or $\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}$, where

$$A[m,n] = \psi_n(\boldsymbol{t}_m).$$

Computational Imaging

There is another important class of linear inverse problems that is mathematically very similar to what is described above, but whose motivation is slightly different.

The basic problem in the field of computational imaging is to recover a function f of one or two or three variables that represents some kind of physical structure indexed by location. Like the regression problems above, we will discretize this problem by representing this function using a basis. Unlike the the regression problems above, we will not observe samples of f, but more general linear functions.

Example: Range profiling using deconvolution

Sending a pulse out (of electromagnetic or acoustic energy) and then listening to the echo is a common way to figure out what is going on in the environment around you. Applications that involve solving a problem of this type are manifold:

- radar imaging
- underwater acoustic imaging
- seismic imaging
- medical imaging
- channel equalization in wireless communications
- image deblurring
- $\cdots$

Mathematically, these problems are set up as follows. We send a known pulse $p(t)$ out, and receive back a signal $y(t)$, which (for physical reasons) is a convolution with another signal $f(t)$:

$$y(t) = \int_{-\infty}^{\infty} f(s)p(t-s)\,\mathrm{d}s.$$

It is this $f(t)$ that we want to recover. You can think of $p(t)$ "bouncing back" to the receiver at many different times with many different weightings — $f(t)$ represents this "reflectivity profile" in time/range.

We can turn this into a discrete matrix problem using a basis expansions for $f(t)$.

Suppose, for example, that $f(t)$ is *time-limited*, in that we know $f(t)$ is zero outside of $[0,T]$. Let $\{\boldsymbol{\psi}_n\}$ be a basis for $L_2([0,T])$. (We have seen many different examples of bases for signals time-limited to an interval.) Truncating this basis to N terms, our model for $f(t)$ is that it can be written as

$$f(t) = \sum_{n=1}^{N} x_n\,\psi_n(t),$$

for some set of expansion coefficients $\boldsymbol{x} \in \mathbb{R}^N$. We can re-write the integral equation above as

$$\begin{aligned} y(t) &= \int_{-\infty}^{\infty} p(t-s) \sum_{n=1}^{N} x_n\,\psi_n(s)\ \mathrm{d}s \\ &= \sum_{n=1}^{N} x_n \left(\int_{-\infty}^{\infty} p(t-s)\,\psi_n(s)\ \mathrm{d}s \right). \end{aligned}$$

In practice, we will in general not observe the continuous-time signal $y(t)$, but rather observe a finite set of **samples** of $y(t)$. Suppose we observe M samples at times $t = t_1, t_2, \ldots, t_M$; for what we are doing here it does not matter whether the samples are equally spaced or not. Now we can write our M observations of $f(t)$ as

$$\begin{aligned} y_m := y(t_m) &= \sum_{n=1}^{N} x_n \left(\int_{-\infty}^{\infty} p(t_m - s)\, \psi_n(s) \ \mathrm{d}s \right) \\ &= \sum_{n} A[m,n]\, x_n \end{aligned}$$

where

$$A[m,n] = \int_{-\infty}^{\infty} p(t_m - s)\, \psi_n(s) \ \mathrm{d}s = \langle \boldsymbol{p}_m, \boldsymbol{\psi}_n \rangle,$$

where $\boldsymbol{p}_m$ is the function

$$p_m(t) = p(t_m - t).$$

If we collect all of the $A[m,n]$ into a $M \times N$ matrix $\boldsymbol{A}$, all of the observations y_m into the vector $\boldsymbol{y} \in \mathbb{R}^M$, and all of the unknown expansion coefficients x_n into the vector $\boldsymbol{x} \in \mathbb{R}^N$, we can write the deconvolution problem as

$$\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}.$$

Again, the solution $\hat{\boldsymbol{x}}$ we get by solving the system of equations above is a vector in $\mathbb{R}^N$, but it specifies as continuous-time signal which we synthesize using

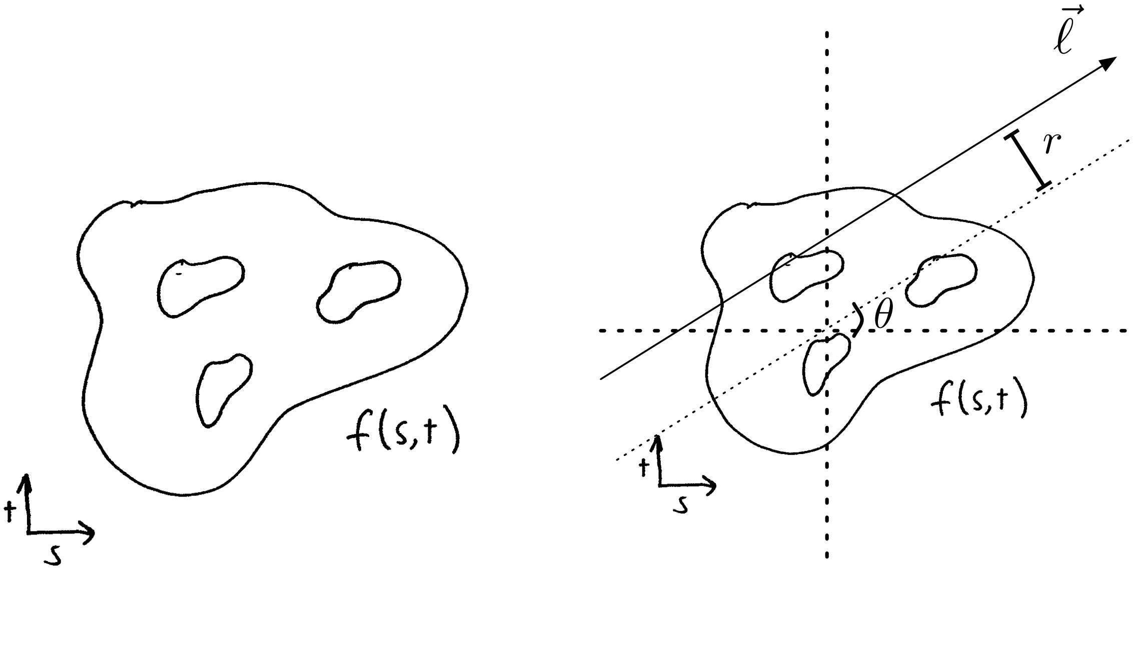
$$\hat{f}(t) = \sum_{n=1}^{N} \hat{x}_n\, \psi_n(t).$$

Example: Tomographic reconstruction

There are many situations where we would like to look inside of an object without have to cut it open. This is particularly true in medical imaging applications, where we would like to get a picture of a person's internal tissue structure in a non-invasive manner.

One method to learn about the interior of an object while only taking measurements on the exterior is **tomography**. When you get a CAT scan on your head, X-rays of a known intensity are emitted on one side of your head, and the intensity is measured as it exits the other side of your head. This is done at many different angles and orientations. The idea is that each of these measurements tells us about the *net absorption* of all the tissues along a narrow path. Below, we will see that a collection of such measurements can be untangled to form a coherent picture of the internal tissue structure.

In the 2D tomographic reconstruction problem, the image $f(s,t)$ we wish to acquire is sampled using line integrals. We can parameterize a line $\vec{\ell}$ using an offset r and an angle θ as shown below:



The line $\vec{\ell}$ is the set of points obeying a linear constraint:

$$\vec{\ell} = \{(s,t) \; : \; -s\sin\theta + t\cos\theta = r\}$$

The integral of $f(s,t)$ along $\vec{\ell}$ is given by

$$\mathscr{R}_{r,\theta}[\boldsymbol{f}] = \begin{cases} \int f\left(s, \frac{r+s\sin\theta}{\cos\theta}\right)\,\mathrm{d}s & |\theta| \leq \pi/4 \\ \int f\left(\frac{t\cos\theta - r}{\sin\theta}, t\right)\,\mathrm{d}t & \pi/4 < |\theta| \leq \pi/2 \end{cases}.$$

Of course, these expressions are equal to one another except when $\theta = 0, \pi/2$. Note also that the measurements are unique only over a range of π, as $\mathscr{R}_{r,\theta+\pi}[\boldsymbol{f}] = \mathscr{R}_{-r,\theta}[\boldsymbol{f}]$.

Given measurements y_m, $m = 1, \ldots, M$ corresponding to line integrals at different different offsets r_m and angles θ_m, which have possibly been corrupted by noise, we would like to estimate the underlying image $f(s,t)$. As above, we will set this up as a linear inverse problem $\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}$.

We start by choosing a finite-dimensional space $\mathcal{F}$ in which to perform the reconstruction that comes equipped with a set of N basis vectors $\{\psi_\gamma(s,t)\}$. We will use the general index $\gamma \in \Gamma$ where Γ is a set of size N as, depending on the basis, it may be convenient to index the basis in different ways (i.e. by integers, pairs of integers over the same range, pairs of integers over different ranges, etc.). For example, if $f(s,t)$ is non-zero only for $(s,t) \in [0,1]^2$, we might take our reconstruction space to be the set of all "pixellated" images — images that are piecewise-constant on squares of side length $1/n$ for some integer n. A natural basis for this space is the set of indicator functions on these squares:

$$\psi_{j,k}(s,t) = \begin{cases} 1 & s \in [j/n, (j+1)/n], \; t \in [k/n, (k+1)/n] \\ 0 & \text{otherwise} \end{cases}$$

Using our general index notation, we can write any $f(s,t) \in \mathcal{F}$ as

$$f(s,t) = \sum_{\gamma \in \Gamma} x_\gamma \psi_\gamma(s,t),$$

where $\Gamma = \{(j,k) \, : \, j,k = 0,1,\ldots,n-1\}$ with size $N = n^2$, and the $x_\gamma \in \mathbb{R}$ are the basis expansion coefficients, which are, in this case, the pixel values. Once again, knowing the discrete set of coefficients x_γ for all $\gamma \in \Gamma$ is the same as knowing the continuous-space function $f(s,t)$.

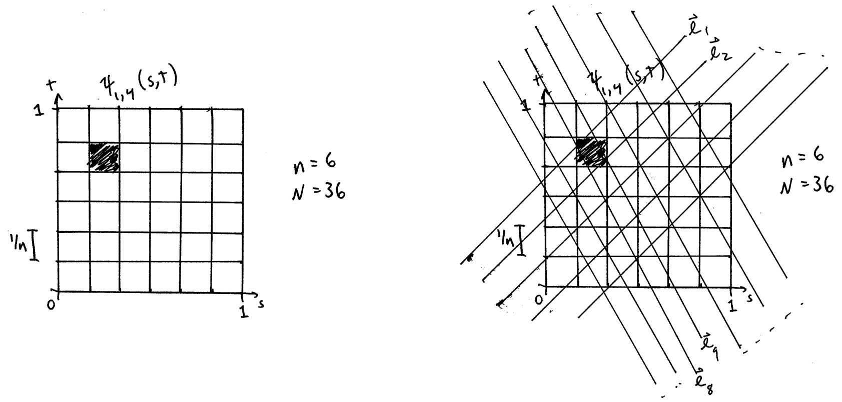
We can also write the measurements of an $f(s,t) \in \mathcal{F}$ in terms of the basis functions:

$$\begin{aligned} y_m &= \mathscr{R}_{r_m,\theta_m}\left[\sum_{\gamma\in\Gamma} x_\gamma \psi_\gamma(s,t)\right] \\ &= \sum_{\gamma\in\Gamma} x_\gamma \mathscr{R}_{r_m,\theta_m}\left[\psi_\gamma(s,t)\right] \qquad \text{(since } \mathscr{R}_{r,\theta}[\cdot] \text{ is linear)} \\ &= \sum_{\gamma\in\Gamma} A[m,\gamma] x_\gamma \qquad \text{where } A[m,\gamma] = \mathscr{R}_{r_m,\theta_m}\left[\psi_\gamma(s,t)\right], \end{aligned}$$

which can be written in more compact form as

$$\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}, \quad A[m,n] = \mathscr{R}_{r_m,\theta_m}[\boldsymbol{\psi}_n], \tag{1}$$

once we put the set Γ in one-to-one correspondence with $\{1,\ldots,N\}$. The action of $\mathscr{R}_{r_m,\theta_m}$ on the basis functions mentioned above (i.e. the quantities we need to compute to form the matrix $\boldsymbol{A}$) is illustrated below. As we can see, not too many of the $\vec{\ell}_m$ pass through a given pixel, meaning that the matrix $\boldsymbol{A}$ will be very sparsely populated.



Left: A sketch of one of the basis functions $\psi_\gamma(s,t)$ from the discussion above. Right: The entries of $\boldsymbol{A}$ in the column indexed by γ will be the result of measuring the basis function $\psi_\gamma(s,t)$: $A[m,\gamma] = \mathscr{R}_{r_m,\theta_m}[\psi_\gamma]$.

Of course, the true underlying image will in general not lie in the chosen finite-dimensional subspace $\mathcal{F}$. This means that even when there is no measurement noise, there will still be some inherent error in our calculations. But solving (1) will in some sense find the member of $\mathcal{F}$ that best explains the measurements that have been observed. If the true image can be closely approximated by a member of $\mathcal{F}$, then we will not lose much through this discretization. A major consideration in choosing the space $\mathcal{F}$ is how well we can use it to approximate images we expect to encounter.

General linear operators

The discretization technique used above for both the $1D$ deconvolution problem and the $2D$ tomographic imaging problem very naturally generalized to different kinds of measurement operators that map signals of a continuous variable(s) into $\mathbb{R}^M$. All we need is that the **functionals** that map the function $f(\boldsymbol{t})$ to the measurements $\{y_m\}$ are **linear**.

Let's make this a little more precise mathematically. As we discussed in the previous lecture, the word "functional" means a mapping from a function to a number — in this case, it is from the underlying function $f(\boldsymbol{t})$ on $\mathbb{R}^D$ to a measurement y_m — we will use[2] $\mathscr{L}_m(\cdot) : \mathcal{S} \rightarrow \mathbb{R}$ to denote these functionals. A **linear functional** simply means that

$$\mathscr{L}_m(\alpha \boldsymbol{f} + \beta \boldsymbol{g}) = \alpha \mathscr{L}_m(\boldsymbol{f}) + \beta \mathscr{L}_m(\boldsymbol{g}), \quad \text{for all} \quad \boldsymbol{f}, \boldsymbol{g} \in \mathcal{S}.$$

Examples of linear functionals include things we have seen above. For instance, sampling at a known location $\boldsymbol{t}_m$,

$$\mathscr{L}_m(\boldsymbol{f}) = f(\boldsymbol{t}_m)$$

and integrating against a known function $\phi_m(t)$

$$\mathscr{L}_m(\boldsymbol{f}) = \int_{-\infty}^{\infty} f(t)\phi_m(t) \ \mathrm{d}t,$$

are both linear functionals. Note that the convolution example above falls into the latter category with $\phi_m(t) = h(t - t_m)$.

[2] Here, $\mathcal{S}$ is a Hilbert space whose members are functions whose domain in $\mathbb{R}^D$; it can be $L_2(\mathbb{R}^D)$, for example

If we have a finite basis decomposition, then discretization works exactly as it did in the special cases above:

$$y_m = \mathscr{L}_m(\boldsymbol{f}) = \mathscr{L}_m\left(\sum_{n=1}^{N} x_n\boldsymbol{\psi}_n\right) = \sum_{n=1}^{N}\mathscr{L}_m(\boldsymbol{\psi}_n)x_n,$$

and so we have the matrix equation

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_M \end{bmatrix} = \begin{bmatrix} \mathscr{L}_1(\boldsymbol{\psi}_1) & \mathscr{L}_1(\boldsymbol{\psi}_2) & \cdots & \mathscr{L}_1(\boldsymbol{\psi}_N) \\ \mathscr{L}_2(\boldsymbol{\psi}_1) & \mathscr{L}_2(\boldsymbol{\psi}_2) & \cdots & \mathscr{L}_2(\boldsymbol{\psi}_N) \\ \vdots & & & \vdots \\ \mathscr{L}_M(\boldsymbol{\psi}_1) & \mathscr{L}_M(\boldsymbol{\psi}_2) & \cdots & \mathscr{L}_M(\boldsymbol{\psi}_N) \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix}$$

or $\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}$. Notice that since the entries of $\boldsymbol{A}$ do not depend on $\boldsymbol{f}$, they can be pre-computed.