

Lecture 22

Constrained vs Unconstrained Formulations

22.1 Lecture Objectives

- Describe the basic types of optimization problems we face, in terms of the presence or absence of constraints.
- Recognize how constraints arise naturally in many optimization applications
- Understand the process by which hard constraints can be approximately included as additional terms in the objective function

22.2 Unconstrained Optimization

An unconstrained optimization problem can be written as follows

$$\text{minimize } f(\mathbf{x}) \tag{22.1}$$

where $\mathbf{x} = [x_1, \dots, x_N]^T \in \mathbb{R}^N$ is the vector we are trying to optimize.

22.3 Constrained Optimization

22.3.1 Hard Constraints

A constrained optimization problem can be written as follows

$$\begin{aligned} &\text{minimize } f(\mathbf{x}) \\ &\text{such that } g_k(\mathbf{x}) \leq b_k, \text{ for } k = 1, \dots, K \\ &\text{such that } h_l(\mathbf{x}) = c_l, \text{ for } l = 1, \dots, L \end{aligned} \tag{22.2}$$

where $\mathbf{x} = [x_1, \dots, x_N]^T \in \mathbb{R}^N$ is the vector we are trying to optimize. However, even though in principle $\mathbf{x}$ can take values all over $\mathbb{R}^N$, in reality it is constrained to the intersection of two regions: the region defined by our inequality constraints ($g_k(\mathbf{x}) \leq b_k$, for $k = 1, \dots, K$), and the region defined by our equality constraints ($h_l(\mathbf{x}) = c_l$, for $l = 1, \dots, L$).

A few comments:

- Equality and inequality constraints arise naturally in a variety of applications. Can you think of a few of each kind?
- Constrained optimization problems are generally a lot harder to solve than unconstrained problems
- General constrained optimization problems can be written in the standard form shown in Equation 22.2 above.

22.3.2 Hard Constraints: Therapy Example

In a typical therapy planning setting, e.g., for intensity-modulated radiation therapy (IMRT), we seek to apply beams of high-energy photons such that a certain spatial dose distribution is achieved. This desire to match a target dose distribution as closely as possible leads naturally to an optimization problem, which is often posed as a least-squares problem. Further, important constraints are often needed in this setting, such as the non-negativity of the fluence map, or potential hard constraints on deposited dose in certain “sensitive” organs (such as the spine) that we need to spare.

The therapy planning problem (focused on “fluence optimization” in this example) can be described as the following constrained formulation:

$$\begin{aligned} \mathbf{x}^* &= \arg \min_{\mathbf{x}} \|\mathbf{D}\mathbf{x} - \mathbf{d}\|_2^2 \\ \text{s.t. } &\mathbf{x} \geq \mathbf{0} \\ &\mathbf{D}_s \mathbf{x} \leq d_{S,max} \end{aligned} \tag{22.3}$$

where $\mathbf{D}$ is the dose deposition matrix mapping the fluence map $\mathbf{x}$ to the dose deposition, which tries to match a desired dose deposition $\mathbf{d}$. The constraints include the basic physical constraint $\mathbf{x} \geq 0$, i.e., that the fluence needs to be non-negative, as well as the hard constraint that the dose deposited in the spine (described by $\mathbf{D}_s \mathbf{x}$, where the matrix $\mathbf{D}_s$ includes the rows of $\mathbf{D}$ corresponding to the target voxels within the spine) needs to be uniformly less than $d_{S,max}$.

Note that this simplified formulation for IMRT therapy planning focuses on the fluence maps, and assumes that all non-negative fluences are feasible. However, ultimately these fluence maps need to be converted to configurations of the multi-leaf collimator. Thus, more advanced versions of therapy planning formulations can include direct aperture optimization, to frame the problem directly in terms of the configurations of the apertures of the multi-leaf collimator (MLC). These formulations may in turn include additional physical constraints (e.g., on the rate of change of MLC apertures). The reading assignments in upcoming homework sets will include reading options describing more sophisticated optimization formulations in the context of therapy planning.

22.3.3 Hard Constraints: Imaging Example

Suppose we are reconstructing an image $\mathbf{x}$ from some data $\mathbf{d} = \mathbf{A}\mathbf{x}$. Further, suppose we know a priori which pixels within the image correspond to tissues (a total of N_T pixels where the image intensity is different from zero), and which pixels correspond to air (a total of N_A pixels where the image intensity is zero). The total number of pixels in the image is $N = N_T + N_A$. This constraint can be expressed as $\mathbf{C}\mathbf{x} = \mathbf{0}$, where $\mathbf{C}$ is a subsampling matrix that selects all the pixels in the air regions (and ignores the rest), and $\mathbf{0}$ is a zero-vector of the appropriate length N_A .

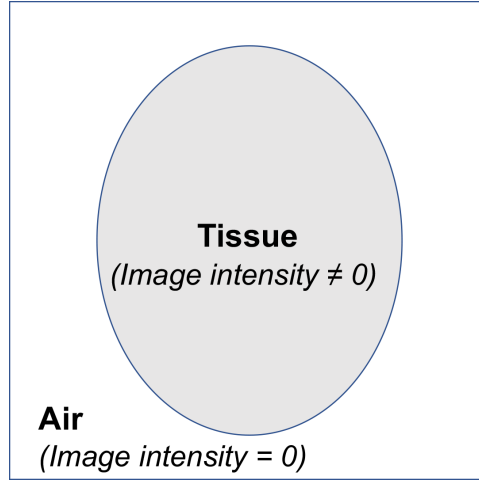


Figure 22.1: Image reconstruction in a case where we know where the air (with image intensity zero) is located.

Putting all these elements together, we have the following constrained formulation:

$$\begin{aligned} \mathbf{x}^* = \arg \min_{\mathbf{x}} \quad & \|\mathbf{A}\mathbf{x} - \mathbf{d}\|_2^2 \\ \text{such that} \quad & \mathbf{C}\mathbf{x} = \mathbf{0} \end{aligned} \quad (22.4)$$

22.3.4 Soft Constraints

A constrained optimization problem (as described above) can be modified to become an unconstrained optimization problem, as follows:

$$\text{minimize } f(\mathbf{x}) + \sum_k \phi_k(g_k(\mathbf{x}) - b_k) + \sum_l \psi_l(h_l(\mathbf{x}) - c_l) \quad (22.5)$$

where ϕ_k is a function that penalizes positive values of its argument, eg: $\phi_k(x) = \lambda_k \max(x, 0)^2$, and ψ_l is a function that penalizes nonzero values of its argument, eg: $\psi_l(x) = \mu_l x^2$. Note that this unconstrained formulation will promote a solution similar to that corresponding to the hard-constraint formulation described above. However, the solutions to Equations [22.2](#) and [22.5](#) are generally not the same.

A few comments:

- How can we pick the functions ϕ_k and ψ_l beyond the (somewhat arbitrary) examples shown above? Note that if we want results very similar to the constrained formulation we are approximating, we may want to pick functions that are zero in the allowed area, and quickly increase towards infinity otherwise. However, this type of very sharp function may not lend itself to easy algorithmic handling (eg: it may not be differentiable everywhere, which can complicate the algorithm).
- The parameters λ_k and μ_k are known as regularization parameters in many applications. These parameters often control the tradeoff between data fidelity and agreement with prior knowledge.

22.3.5 Soft Constraints: Therapy Example

The IMRT therapy planning formulation with spine-sparing hard constraints ($\mathbf{D}_s \mathbf{x} \leq d_{S,max}$) described above (Eq. 22.3) can be converted into a problem where these constraints are included into the cost function, as soft constraints:

$$\begin{aligned} \mathbf{x}^* &= \arg \min_{\mathbf{x}} \|\mathbf{D}\mathbf{x} - \mathbf{d}\|_2^2 + w \|(\mathbf{D}_s \mathbf{x} - d_{S,max})_+\|^2 \\ \text{s.t. } &\mathbf{x} \geq \mathbf{0} \end{aligned} \quad (22.6)$$

where the operation $(\mathbf{y})_+$ performs the element-wise operation $\max(y_m, 0)$ on the elements of $\mathbf{y}$. In other words, the additional cost function term $w \|(\mathbf{D}_s \mathbf{x} - d_{S,max})_+\|^2$ penalizes dose deposition in the spine exceeding a certain value $d_{S,max}$ without expressly forbidding it. The quadratic form of this expression indicates that spinal dose deposition slightly above $d_{S,max}$ will be penalized lightly, whereas spinal dose deposition substantially above $d_{S,max}$ will be penalized heavily. The parameter w controls the relative weight of this spinal dose penalty (i.e., very low values of w largely disregard this desired constraint, whereas very high values of w lead to essentially a hard constraint as described previously in Eq. 22.3). In this example, the basic physical constraint that $\mathbf{x} \geq \mathbf{0}$ has been maintained in the formulation as a hard constraint, as violations of this constraint would lead to non-physical solutions.

22.3.6 Soft Constraints: Imaging Example

The example above (Section 22.3.3) applied hard constraints to an image reconstruction problem, and forced the pixel values to be zero in the image regions known to be air. A related approach to pose the reconstruction problem is to apply a soft constraint. In this case, instead of forcing the pixel values to be zero in the air regions, we can “encourage” small pixel values in this regions. For example, one might pose the reconstruction as follows:

$$\mathbf{x}^* = \arg \min_{\mathbf{x}} \|\mathbf{A}\mathbf{x} - \mathbf{d}\|_2^2 + \lambda \|\mathbf{C}\mathbf{x}\|_2^2 \quad (22.7)$$

for some value of $\lambda > 0$. Note that the last term in our formulation will result in a penalty for non-zero values of the image in the air region, but it will not penalize non-zero values

in the tissue region. Further, this soft formulation will lead to higher penalty for higher values in the air region, whereas the hard constraint formulation above directly forbids any non-zero values, regardless of the specifics.

Question: What will happen to this soft constraint formulation if we set λ very small ($\lambda \rightarrow 0$)? How about if λ is very large ($\lambda \rightarrow \infty$)?

