

# Chapter 7

## Optimization and Minimum Principles

### 7.1 Two Fundamental Examples

Within the universe of applied mathematics, optimization is often a world of its own. There are occasional expeditions to other worlds (like differential equations), but mostly the life of optimizers is self-contained: *Find the minimum of  $F(x_1, \dots, x_n)$* . That is not an easy problem, especially when there are many variables  $x_j$  and many constraints on those variables. *Those constraints may require  $Ax = b$  or  $x_j \geq 0$  or both or worse*. Whole books and courses and software packages are dedicated to this problem of *constrained minimization*.

I hope you will forgive the poetry of worlds and universes. I am trying to emphasize the importance of optimization—a key component of engineering mathematics and scientific computing. This chapter will have its own flavor, but it is strongly connected to the rest of this book. To make those connections, I want to begin with two specific examples. **If you read even just this section**, you will see the connections.

#### Least Squares

Ordinary least squares begins with a matrix  $A$  whose  $n$  columns are independent. The rank is  $n$ , so  $A^T A$  is symmetric positive definite. The input vector  $b$  has  $m$  components, the output  $\hat{u}$  has  $n$  components, and  $m > n$ :

<b>Least squares problem</b> <b>Normal equations for best <math>\hat{u}</math></b>	$\begin{aligned} &\text{Minimize } \ Au - b\ ^2 \\ &A^T A \hat{u} = A^T b \end{aligned}$	(1)
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Those equations  $A^T A \hat{u} = A^T b$  say that the error residual  $e = b - A\hat{u}$  solves  $A^T e = 0$ . Then  $e$  is perpendicular to columns 1, 2,  $\dots$ ,  $n$  of  $A$ . Write those zero inner products

as  $(\text{column})^T(e) = 0$  to find  $A^T A \hat{u} = A^T b$ :

$$\begin{bmatrix} (\text{column } 1)^T \\ \vdots \\ (\text{column } n)^T \end{bmatrix} \begin{bmatrix} e \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix} \quad \text{is} \quad \begin{aligned} A^T e &= 0 \\ A^T(b - A\hat{u}) &= 0 \\ A^T A \hat{u} &= A^T b. \end{aligned} \quad (2)$$

Graphically, Figure 7.1 shows  $A\hat{u}$  as the *projection of  $b$* . It is the combination of columns of  $A$  (the point in the column space) that is nearest to  $b$ . We studied least squares in Section 2.3, and now we notice that **a second problem is solved at the same time**.

This second problem (*dual problem*) does not project  $b$  down onto the column space. Instead it projects  $b$  across onto the perpendicular space. In the 3D picture, that space is a line (its dimension is  $3 - 2 = 1$ ). In  $m$  dimensions that perpendicular subspace has dimension  $m - n$ . *It contains the vectors that are perpendicular to all columns of  $A$* . The line in Figure 7.1 is the **nullspace of  $A^T$** .

One of the vectors in that perpendicular space is  $e =$  projection of  $b$ ! Together,  $e$  and  $\hat{u}$  solve the two linear equations that express exactly what the figure shows:

<b>Primal-Dual</b>	$e + A\hat{u} = b$	$m$ equations	(3)
<b>Saddle Point</b>	$A^T e = 0$	$n$ equations	
<b>Kuhn-Tucker (KKT)</b>			

We took this chance to write down three names for these very simple but so fundamental equations. I can quickly say a few words about each name.

**Primal-Dual** The primal problem is to minimize  $\|Au - b\|^2$ . This produces  $\hat{u}$ . The dual problem is to minimize  $\|w - b\|^2$ , under the condition that  $A^T w = 0$ . This produces  $e$ . We can't solve one problem without solving the other. They are solved together by equation (3), which finds the projections in both directions.

**Saddle Point** The block matrix  $S$  in those equations is not positive definite!

**Saddle point matrix** (4)

$$S = \begin{bmatrix} I & A \\ A^T & 0 \end{bmatrix}$$

The first  $m$  pivots are all 1's, from the matrix  $I$ . When elimination puts zeros in place of  $A^T$ , *it puts the negative definite  $-A^T A$  into the zero block*.

**Multiply row 1 by  $A^T$**   
**Subtract from row 2**

$$\begin{bmatrix} I & 0 \\ -A^T & I \end{bmatrix} \begin{bmatrix} I & A \\ A^T & 0 \end{bmatrix} = \begin{bmatrix} I & A \\ 0 & -A^T A \end{bmatrix}. \quad (5)$$

That elimination produced  $-A^T A$  in the  $(2, 2)$  block (the "Schur complement"). So the final  $n$  pivots will all be negative.  $S$  is **indefinite**, with pivots of both signs.

$S$  doesn't produce a pure minimum or maximum, positive or negative definite. It leads to a saddle point  $(\hat{u}, e)$ . When we get up more courage, we will try to draw this.

**Kuhn-Tucker** These are the names most often associated with equations like (3) that solve optimization problems. Because of an earlier Master’s Thesis by Karush, you often see “KKT equations.” In continuous problems, for functions instead of vectors, the right name would be “Euler-Lagrange equations.” When the constraints include inequalities like  $w \geq 0$  or  $Bu = d$ , Lagrange multipliers are still the key. For those more delicate problems, Kuhn and Tucker earned their fame.

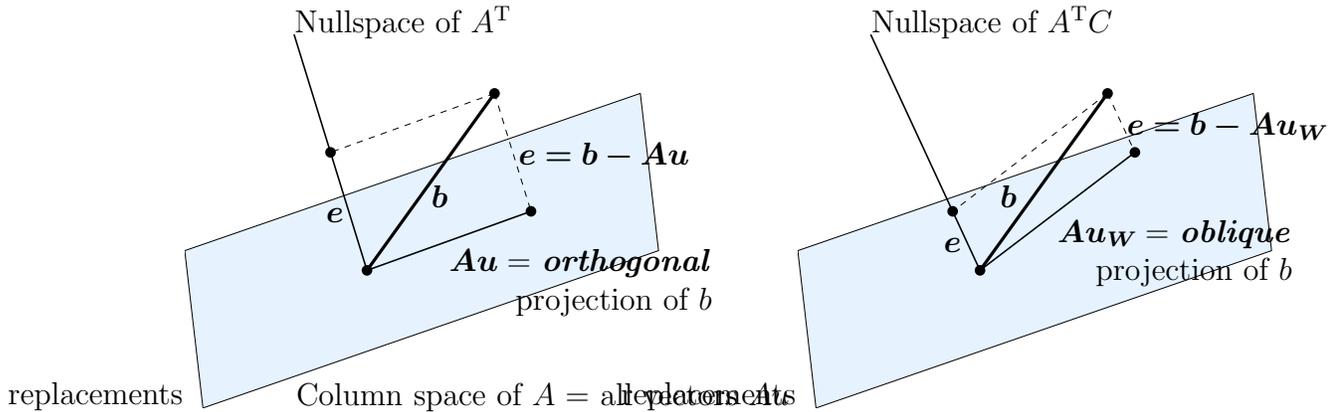


Figure 7.1: Ordinary and weighted least squares:  $\min \|b - Au\|^2$  and  $\|Wb - WAu\|^2$ .

### Weighted Least Squares

This is a small but very important extension of the least squares problem. It involves the same rectangular  $A$ , and a square weighting matrix  $W$ . Instead of  $\hat{u}$  we write  $\hat{u}_W$  (this best answer changes with  $W$ ). You will see that the symmetric positive definite combination  $C = W^T W$  is what matters in the end.

<b>Weighted least squares</b> <b>Normal equations for <math>\hat{u}_W</math></b>	Minimize $\ WAu - Wb\ ^2$ $(WA)^T(WA)\hat{u}_W = (WA)^T(Wb)$	(6)
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No new mathematics, just replace  $A$  and  $b$  by  $WA$  and  $Wb$ . The equation has become  $A^T W^T W A \hat{u}_W = A^T W^T W b$  or  $A^T C A \hat{u}_W = A^T C b$  or  $A^T C (b - A \hat{u}_W) = 0$ . (7)

In the middle equation is that all-important matrix  $A^T C A$ . In the last equation,  $A^T e = 0$  has changed to  $A^T C e = 0$ . When I made that change in Figure 7.1, I lost the  $90^\circ$  angles. The line is no longer perpendicular to the plane, and the projections are no longer orthogonal. We are still splitting  $b$  into two pieces,  $A \hat{u}_W$  in the column space and  $e$  in the nullspace of  $A^T C$ . The equations now include this  $C = W^T W$ :

<b><math>e</math> is “<math>C</math>-orthogonal” to the columns of <math>A</math></b>	$\begin{aligned} e + A \hat{u}_W &= b \\ A^T C e &= 0 \end{aligned}$	(8)
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With a simple change, the equations (8) become symmetric! **Introduce  $w = Ce$  and  $e = C^{-1}w$  and shorten  $\hat{u}_W$  to  $u$ :**

Primal-Dual  
Saddle Point  
Kuhn-Tucker

$$\begin{aligned} C^{-1}w + Au &= b \\ A^T w &= 0 \end{aligned} \quad (9)$$

This weighted saddle point matrix replaces  $I$  by  $C^{-1}$  (still symmetric):

Saddle point matrix

$$S = \begin{bmatrix} -1 & A \\ A^T & 0 \end{bmatrix} \begin{matrix} m \text{ rows} \\ n \text{ rows} \end{matrix}$$

Elimination produces  $m$  positive pivots from  $C^{-1}$ , and  $n$  negative pivots from  $-A^T C A$ :

$$\begin{bmatrix} C^{-1} & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} w \\ u \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix} \longleftrightarrow \begin{bmatrix} C^{-1} & A \\ 0 & -A^T C A \end{bmatrix} \begin{bmatrix} w \\ u \end{bmatrix} = \begin{bmatrix} b \\ -A^T C b \end{bmatrix}. \quad (10)$$

The “Schur complement” that appears in the 2,2 block becomes  $-A^T C A$ . We are back to  $A^T C A u = A^T C b$  and all its applications.

Two more steps will finish this overview of optimization. We show how a different vector  $f$  can appear on the right side. The bigger step is also taken by our second example, coming now. *The dual problem (for  $w$  not  $u$ ) has a constraint.* At first it was  $A^T e = 0$ , now it is  $A^T w = 0$ , and in the example it will be  $A^T w = f$ .

**How do you minimize a function of  $e$  or  $w$  when these constraints are enforced?** Lagrange showed the way, with his multipliers.

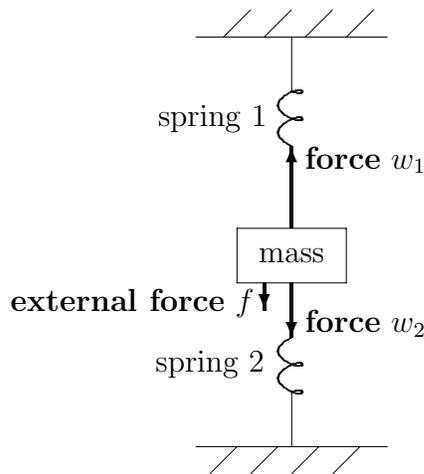
## Minimizing with Constraints

The second example is a line of *two springs and one mass*. The function to minimize is the energy in the springs. The constraint is the balance  $A^T w = f$  between internal forces (in the springs) and the external force (on the mass). I believe you can see in Figure 7.2 the fundamental problem of constrained optimization. The forces are drawn as if both springs are stretched with forces  $f > 0$ , pulling on the mass. Actually spring 2 will be compressed ( $w_2$  is negative).

As I write those words—*spring, mass, energy, force balance*—I am desperately hoping that you won’t just say “this is not my area.” Changing the example to another area of science or engineering or economics would be easy, the problem stays the same in all languages.

All of calculus trains us to minimize functions: **Set the derivative to zero!** But the basis calculus course doesn’t deal properly with constraints. We are minimizing an energy function  $E(w_1, w_2)$ , but we are constrained to stay on the line  $w_1 - w_2 = f$ . *What derivatives do we set to zero?*

A direct approach is to solve the constraint equation. Replace  $w_2$  by  $w_1 - f$ . That seems natural, but I want to advocate a different approach (which leads to the same result). Instead of looking for  $w$ ’s that satisfy the constraint, the idea of Lagrange is



**Internal energy in the springs**

$$E(w) = E_1(w_1) + E_2(w_2)$$

**Balance of internal/external forces**

$$w_1 - w_2 = f \quad (\text{the constraint})$$

**Constrained optimization problem**

Minimize  $E(w)$  subject to  $w_1 - w_2 = f$

Figure 7.2: Minimum spring energy  $E(w)$  subject to balance of forces.

to *build the constraints into the function*. Rather than removing  $w_2$ , we will add a new unknown  $u$ . It might seem surprising, but this second approach is better.

With  $n$  constraints on  $m$  unknowns, Lagrange's method has  $m+n$  unknowns. The idea is to add a **Lagrange multiplier** for each constraint. (Books on optimization call this multiplier  $\lambda$  or  $\pi$ , we will call it  $u$ .) Our Lagrange function  $L$  has the constraint  $w_1 - w_2 - f = 0$  built in, and multiplied by  $-u$ :

<b>Lagrange function</b>	$L(w_1, w_2, u) = E_1(w_1) + E_2(w_2) - u(w_1 - w_2 - f).$
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Calculus can operate on  $L$ , by setting derivatives (*three partial derivatives!*) to zero:

<b>Kuhn-Tucker optimality equations</b>	$\frac{\partial L}{\partial w_1} = \frac{dE_1}{dw}(w_1) - u = 0$	(11a)
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	$\frac{\partial L}{\partial w_2} = \frac{dE_2}{dw}(w_2) + u = 0$	(11b)
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<b>Lagrange multiplier <math>u</math></b>	$\frac{\partial L}{\partial u} = -(w_1 - w_2 - f) = 0$	(11c)
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Notice how the third equation  $\partial L/\partial u = 0$  automatically brings back the constraint—because it was just multiplied by  $-u$ . If we add the first two equations to eliminate  $u$ , and substitute  $w_1 - f$  for  $w_2$ , we are back to the direct approach with one unknown.

But we don't want to eliminate  $u$ ! That Lagrange multiplier is an important number with a meaning of its own. In this problem,  $u$  is the displacement of the mass. In economics,  $u$  is the selling price to maximize profit. In all problems,  $u$  measures the **sensitivity of the answer** (the minimum energy  $E_{\min}$ ) to a change in the constraint. We will see this sensitivity  $dE_{\min}/df$  in the linear case.

## Linear Case

The force in a linear spring is proportional to the elongation  $e$ , by Hooke's Law  $w = ce$ . Each small stretching step requires work = (force)(movement) =  $(ce)(\Delta e)$ . Then the integral  $\frac{1}{2}ce^2$  that adds up those small steps gives the energy stored in the spring. We can express this energy in terms of  $e$  or  $w$ :

**Energy in a spring**  $E(w) = \frac{1}{2}ce^2 = \frac{1}{2}\frac{w^2}{c}$ . (12)

Our problem is to minimize a quadratic energy  $E(w)$  subject to a linear balance equation  $w_1 - w_2 = f$ . This is the model problem of optimization.

**Minimize**  $E(w) = \frac{1}{2}\frac{w_1^2}{c_1} + \frac{1}{2}\frac{w_2^2}{c_2}$  **subject to**  $w_1 - w_2 = f$ . (13)

We want to solve this model problem by geometry and then by algebra.

**Geometry** In the plane of  $w_1$  and  $w_2$ , draw the line  $w_1 - w_2 = f$ . Then draw the ellipse  $E(w) = E_{\min}$  that *just touches this line*. The line is tangent to the ellipse. A smaller ellipse from smaller forces  $w_1$  and  $w_2$  will not reach the line—those forces will not balance  $f$ . A larger ellipse will not give minimum energy. This ellipse touches the line at the point  $(w_1, w_2)$  that minimizes  $E(w)$ .

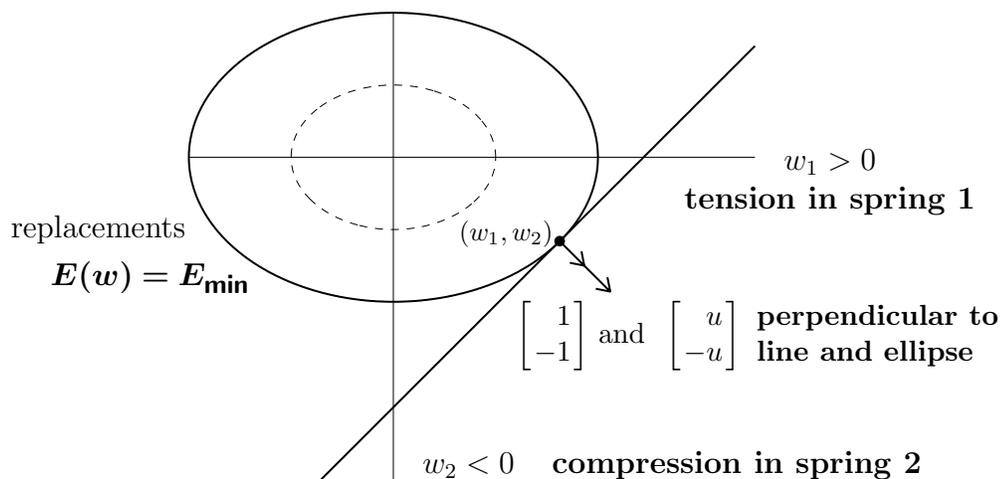


Figure 7.3: The ellipse  $E(w) = E_{\min}$  touches  $w_1 - w_2 = f$  at the solution  $(w_1, w_2)$ .

At the touching point in Figure 7.3, the perpendiculars  $(1, -1)$  and  $(u, -u)$  to the line and the ellipse are parallel. The perpendicular to the line is the vector  $(1, -1)$  from the partial derivatives of  $w_1 - w_2 = f$ . The perpendicular to the ellipse is  $(\partial E/\partial w_1, \partial E/\partial w_2)$ , from the gradient of  $E(w)$ . By the optimality equations (11a) and (11b), this is exactly  $(u, -u)$ . Those parallel gradients at the solution are the algebraic statement that **the line is tangent to the ellipse**.

**Algebra** To find  $(w_1, w_2)$ , start with the derivatives of  $w_1^2/2c_1$  and  $w_2^2/2c_2$ :

$$\text{Energy gradient} \quad \frac{\partial E}{\partial w_1} = \frac{w_1}{c_1} \quad \text{and} \quad \frac{\partial E}{\partial w_2} = \frac{w_2}{c_2}. \quad (14)$$

Equations (11a) and (11b) in Lagrange's method become  $w_1/c_1 = u$  and  $w_2/c_2 = -u$ . Now the constraint  $w_1 - w_2 = f$  yields  $(c_1 + c_2)u = f$  (both  $w$ 's are eliminated):

$$\text{Substitute } w_1 = c_1 u \text{ and } w_2 = -c_2 u. \text{ Then } (c_1 + c_2)u = f. \quad (15)$$

I don't know if you recognize  $c_1 + c_2$  as our stiffness matrix  $A^T C A$ ! This problem is so small that you could easily miss  $K = A^T C A$ . The matrix  $A^T$  in the constraint equation  $A^T w = w_1 - w_2 = f$  is only 1 by 2, so *the stiffness matrix  $K$  is 1 by 1*:

$$A^T = [1 \quad -1] \quad \text{and} \quad K = A^T C A = [1 \quad -1] \begin{bmatrix} c_1 & \\ & c_2 \end{bmatrix} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = [c_1 + c_2]. \quad (16)$$

The algebra of Lagrange's method has recovered  $Ku = f$ . Its solution is the movement  $u = f/(c_1 + c_2)$  of the mass. Equation (15) eliminated  $w_1$  and  $w_2$  using (11a) and (11b). Now back substitution finds those energy-minimizing forces:

$$\text{Spring forces} \quad w_1 = c_1 u = \frac{c_1 f}{c_1 + c_2} \quad \text{and} \quad w_2 = -c_2 u = \frac{-c_2 f}{c_1 + c_2}. \quad (17)$$

Those forces  $(w_1, w_2)$  are on the ellipse of minimum energy  $E_{\min}$ , tangent to the line:

$$E(w) = \frac{1}{2} \frac{w_1^2}{c_1} + \frac{1}{2} \frac{w_2^2}{c_2} = \frac{1}{2} \frac{c_1 f^2}{(c_1 + c_2)^2} + \frac{1}{2} \frac{c_2 f^2}{(c_1 + c_2)^2} = \frac{1}{2} \frac{f^2}{c_1 + c_2} = E_{\min}. \quad (18)$$

This  $E_{\min}$  must be the same minimum value  $\frac{1}{2} f^T K^{-1} f$  as in Section \_\_\_\_\_. It is.

We can directly verify the mysterious fact that  $u$  measures the sensitivity of  $E_{\min}$  to a small change in  $f$ . Compute the derivative  $dE_{\min}/df$ :

$$\text{Lagrange multiplier} = \text{Sensitivity} \quad \frac{d}{df} \left( \frac{1}{2} \frac{f^2}{c_1 + c_2} \right) = \frac{f}{c_1 + c_2} = u. \quad (19)$$

This sensitivity is linked to the observation in Figure 7.3 that one gradient is  $u$  times the other gradient. From (11a) and (11b), that stays true for nonlinear springs.

## A Specific Example

I want to insert  $c_1 = c_2 = 1$  in this model problem, to see the saddle point of  $L$  more clearly. The Lagrange function with built-in constraint depends on  $w_1$  and  $w_2$  and  $u$ :

$$L = \frac{1}{2} w_1^2 + \frac{1}{2} w_2^2 - u w_1 + u w_2 + u f. \quad (20)$$

The equations  $\partial L/\partial w_1 = 0$  and  $\partial L/\partial w_2 = 0$  and  $\partial L/\partial u = 0$  produce a beautiful symmetric saddle-point matrix  $S$ :

$$\begin{aligned} \partial L/\partial w_1 &= w_1 - u = 0 \\ \partial L/\partial w_2 &= w_2 + u = 0 \\ \partial L/\partial u &= -w_1 + w_2 = f \end{aligned} \quad \text{or} \quad \begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & 1 \\ -1 & 1 & 0 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ u \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ f \end{bmatrix}. \quad (21)$$

Is this matrix  $S$  positive definite? *No.* It is invertible, and its pivots are 1, 1,  $-2$ . That  $-2$  destroys positive definiteness—it means a saddle point:

**Elimination**  $\begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & 1 \\ -1 & 1 & 0 \end{bmatrix} \longrightarrow \begin{bmatrix} 1 & 0 & -1 \\ & 1 & 1 \\ & & -2 \end{bmatrix}$  with  $L = \begin{bmatrix} 1 & & \\ & 1 & \\ & & 1 \end{bmatrix}$ .

On a symmetric matrix, elimination equals “completing the square.” The pivots 1, 1,  $-2$  are outside the squares. The entries of  $L$  are inside the squares:

$$\frac{1}{2}w_1^2 + \frac{1}{2}w_2^2 - uw_1 + uw_2 = \frac{1}{2} [1(w_1 - u)^2 + 1(w_2 + u)^2 - 2(u)^2]. \quad (22)$$

The first squares  $(w_1 - u)^2$  and  $(w_2 + u)^2$  go “upwards,” but  $-2u^2$  goes down. **This gives a saddle point SP =  $(w_1, w_2, u)$  in Figure 7.4.**

The eigenvalues of a symmetric matrix have the same signs as the pivots, and the same product (which is  $\det S = -2$ ). Here the eigenvalues are  $\lambda = 1, 2, -1$ .

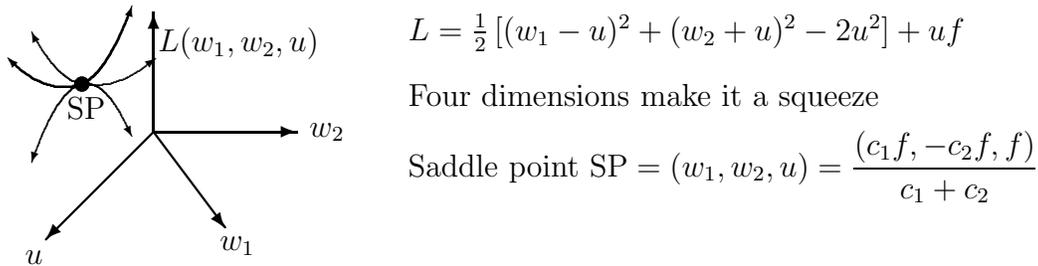


Figure 7.4:  $(w_1 - u)^2$  and  $(w_2 + u)^2$  go up,  $-2u^2$  goes down from the saddle point SP.

## The Fundamental Problem

May I describe the full linear case with  $w = (w_1, \dots, w_m)$  and  $A^T w = (f_1, \dots, f_n)$ ? The problem is to minimize the total energy  $E(w) = \frac{1}{2} w^T C^{-1} w$  in the  $m$  springs. The  $n$  constraints  $A^T w = f$  are built in by Lagrange multipliers  $u_1, \dots, u_n$ . Multiplying the force balance on the  $k$ th mass by  $-u_k$  and adding, all  $n$  constraints are built into the dot product  $u^T (A^T w - f)$ . For mechanics, we use a minus sign in  $L$ :

**Lagrange function**  $L(w, u) = \frac{1}{2} w^T C^{-1} w - u^T (A^T w - f). \quad (23)$

To find the minimizing  $w$ , set the  $m + n$  first partial derivatives of  $L$  to zero:

$$\begin{array}{l} \mathbf{Kuhn-Tucker} \\ \mathbf{optimality} \end{array} \quad \partial L / \partial w = C^{-1}w - Au = 0 \quad (24a)$$

$$\begin{array}{l} \mathbf{equations} \end{array} \quad \partial L / \partial u = -A^T w + f = 0 \quad (24b)$$

This is the main point, that Lagrange multipliers lead exactly to the linear equations  $w = CAu$  and  $A^T w = f$  that we studied in the first chapters of the book. By using  $-u$  in the Lagrange function  $L$  and introducing  $e = Au$ , we have the plus signs that appeared for springs and masses:

$$e = Au \quad w = Ce \quad f = A^T w \quad \implies \quad A^T CAu = f.$$

**Important** Least squares problems have  $e = b - Au$  (minus sign from voltage drops). **Then we change to  $+u$  in  $L$ .** The energy  $E = \frac{1}{2}w^T C^{-1}w - b^T w$  now has a term involving  $b$ . When Lagrange sets derivatives of  $L$  to zero, he finds  $S!$

$$\begin{array}{l} \partial L / \partial w = C^{-1}w + Au - b = 0 \\ \partial L / \partial u = A^T w - f = 0 \end{array} \quad \text{or} \quad \begin{bmatrix} C^{-1} & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} w \\ u \end{bmatrix} = \begin{bmatrix} b \\ f \end{bmatrix}. \quad (25)$$

This system is my top candidate for the fundamental problem of scientific computing.

You could eliminate  $w = C(b - Au)$  *but I don't know if you should*. If you do it,  $K = A^T CA$  will appear. Usually this is a good plan:

$$\mathbf{Remove } w \quad A^T w = A^T C(b - Au) = f \quad \text{which is} \quad A^T CAu = A^T Cb - f. \quad (26)$$

## Duality and Saddle Points

We minimize the energy  $E(w)$  but we do *not* minimize Lagrange's function  $L(w, u)$ . It is true that  $\partial L / \partial w$  and  $\partial L / \partial u$  are zero at the solution. But the matrix of second derivatives of  $L$  is not positive definite. **The solution  $w, u$  is a saddle point.** It is a minimum of  $L$  over  $w$ , and at the same time it is a maximum of  $L$  over  $u$ . A saddle point has something to do with a horse... It is like the lowest point in a mountain range, which is also the highest point as you go across.

The *minimax theorem* states that we can minimize first (over  $w$ ) or maximize first (over  $u$ ). Either order leads to the unique saddle point, given by  $\partial L / \partial w = 0$  and  $\partial L / \partial u = 0$ . The minimization removes  $w$  from the problem, and it corresponds exactly to eliminating  $w$  from the equations (11) for "first derivatives = 0." Every step will be illustrated by examples (linear case first).

Allow me to use the  $A, C, A^T$  notation that we already know, so I can point out the fantastic idea of **duality**. The Lagrangian is  $L(w, u) = \frac{1}{2}w^T C^{-1}w - u^T (A^T w - f)$ , leaving out  $b$  for simplicity. We compare minimization first and maximization first:

**Minimize over  $w$**   $\partial L/\partial w = 0$  when  $C^{-1}w - Au = 0$ . Then  $w = CAu$  and  $L = -\frac{1}{2}(Au)^T C(Au) + u^T f$ . This is to be maximized.

**Maximize over  $u$**  Key point:  $L_{\max} = +\infty$  if  $A^T w \neq f$ . Minimizing over  $w$  will keep  $A^T w = f$  to avoid that  $+\infty$ . Then  $L = \frac{1}{2}w^T C^{-1}w$ .

The maximum of a linear function like  $5u$  is  $+\infty$ . But the maximum of  $0u$  is 0.

Now come the two second steps, maximize over  $u$  and minimize over  $w$ . **Those are the dual problems.** Often one problem is called the “primal” and the other is its “dual”—but they are reversible. Here are the two dual principles for linear springs:

1. Choose  $u$  to maximize  $-\frac{1}{2}(Au)^T C(Au) + u^T f$ . Call this function  $-P(u)$ .
2. Choose  $w$  to minimize  $\frac{1}{2}w^T C^{-1}w$  keeping the force balance  $A^T w = f$ .

Our original problem was **2**. In the language of mechanics, we were minimizing the complementary energy  $E(w)$ . Its dual problem is **1**. This minimizes the potential energy  $P(u)$ , by maximizing  $-P(u)$ . Most finite element systems choose that “displacement method.” They work with  $u$  because it avoids the constraint  $A^T w = f$ .

The dual problems **1** and **2** involve the same inputs  $A, C, f$  but they look entirely different. *Equality between  $\min_{\max}(L)$  and  $\max_{\min}(L)$  gives the duality principle and the saddle point:*

$$\text{Duality of 1 and 2} \quad \max_{\text{all } u} (-P(u)) = \min_{A^T w = f} E(w). \quad (27)$$

That is the big theorem of optimization—the **maximum of one problem equals the minimum of its dual**. We can find those numbers, and see that they are equal, because the derivatives are linear. Maximizing  $-P(u)$  will minimize  $P(u)$ , which is the problem we solved in Chapter 1. Write  $u^*$  and  $w^*$  for the minimizer and maximizer:

1.  $P(u) = \frac{1}{2}u^T A^T C A u - u^T f$  is  $P_{\min} = -\frac{1}{2}f^T (A^T C A)^{-1} f$  when  $u^* = (A^T C A)^{-1} f$
2.  $E(w) = \frac{1}{2}w^T C^{-1} w$  is  $E_{\min} = \frac{1}{2}f^T (A^T C A)^{-1} f$  when  $w^* = C A u^*$ .

So  $u^* = K^{-1} f$  and  $w^* = C A u^*$  give the saddle point  $(w^*, u^*)$  of  $L$ . This is where  $E_{\min} = -P_{\min}$ .

### Problem Set 7.1

- 1 Our model matrix  $M$  in (21) has eigenvalues  $\lambda_1 = 1, \lambda_2 = 2, \lambda_3 = -1$ :

$$M = \begin{bmatrix} C^{-1} & A \\ A^T & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & 1 \\ -1 & 1 & 0 \end{bmatrix}$$

The trace  $1 + 1 + 0$  down the diagonal of  $M$  equals the sum of  $\lambda$ 's. Check that  $\det M = \text{product of } \lambda$ 's. Find eigenvectors  $x_1, x_2, x_3$  of unit length for those eigenvalues  $1, 2, -1$ . The eigenvectors are orthogonal!

**2** The quadratic part of the Lagrangian  $L(w_1, w_2, u)$  comes directly from  $M$ :

$$\frac{1}{2} \begin{bmatrix} w_1 & w_2 & u \end{bmatrix} \begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & 1 \\ -1 & 1 & 0 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ u \end{bmatrix} = \frac{1}{2} (w_1^2 + w_2^2 - 2uw_1 + 2uw_2).$$

Put the unit eigenvectors  $x_1, x_2, x_3$  inside the squares and  $\lambda = 1, 2, -1$  outside:

$$w_1^2 + w_2^2 - 2uw_1 + 2uw_2 = 1(\text{---})^2 + 2(\text{---})^2 - 1(\text{---})^2.$$

The first parentheses contain  $(1w_1 - 1w_2 + 0w_3)/\sqrt{2}$  because  $x_1$  is  $(1, -1, 0)/\sqrt{2}$ . Compared with (22), these squares come from orthogonal eigenvector directions. We are using  $A = Q\Lambda Q^T$  instead of  $A = LDL^T$ .

**3** *Weak duality* Half of the duality theorem is  $\max -P(u) \leq \min E(w)$ . This is surprisingly easy to prove. Show that  $-P(u)$  is *always smaller* than  $E(w)$ , for every  $u$  and  $w$  with  $A^T w = f$ .

$$-\frac{1}{2}u^T A^T C A u + u^T f \leq \frac{1}{2}w^T C^{-1} w \quad \text{whenever } A^T w = f.$$

Set  $f = A^T w$ . Verify that (right side)  $-$  (left side)  $= \frac{1}{2}(w - CAu)^T C^{-1}(w - CAu) \geq 0$ .

Equality holds and  $\max(-P) = \min(E)$  when  $w = CAu$ . That is equation (11)!

**4** Suppose the lower spring in Figure 7.2 is not fixed at the bottom. A mass at that end adds a new force balance constraint  $w_2 - f_2 = 0$ . Build the old and new constraints into the Lagrange function  $L(w_1, w_2, u_1, u_2)$  to minimize the energy  $E_1(w_1) + E_2(w_2)$ . Write down *four equations* like (11a)–(11c): partial derivatives of  $L$  are zero.

**5** For spring energies  $E_1 = \frac{1}{2}w_1^2/c_1$  and  $E_2 = \frac{1}{2}w_2^2/c_2$ , find  $A$  in the block form

$$\begin{bmatrix} C^{-1} & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} w \\ u \end{bmatrix} = \begin{bmatrix} 0 \\ f \end{bmatrix} \quad \text{with } w = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}, u = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}, f = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix}.$$

Elimination subtracts  $A^T C$  times the first block row from the second. With  $c_1 = c_2 = 1$ , what matrix  $-A^T C A$  enters the zero block? Solve for  $u = (u_1, u_2)$ .

**6** Continuing Problem 5 with  $C = I$ , write down  $w = CAu$  and compute the energy  $E_{\min} = \frac{1}{2}w_1^2 + \frac{1}{2}w_2^2$ . Verify that its derivatives with respect to  $f_1$  and  $f_2$  are the Lagrange multipliers  $u_1$  and  $u_2$  (sensitivity analysis).

## Solutions 7.1

4. The Lagrange function is  $L = E_1(w_1) + E_2(w_2) - u_1(w_1 - w_2 - f_1) - u_2(w_2 - f_2)$ .  
Its first partial derivatives at the saddle point are

$$\begin{aligned}\frac{\partial L}{\partial w_1} &= \frac{dE_1}{dw}(w_1) - u_1 = 0 \\ \frac{\partial L}{\partial w_2} &= \frac{dE_2}{dw}(w_2) + u_1 - u_2 = 0 \\ \frac{\partial L}{\partial u_1} &= -(w_1 - w_2 - f_1) = 0 \\ \frac{\partial L}{\partial u_2} &= -(w_2 - f_2) = 0.\end{aligned}$$

$$5. \begin{bmatrix} C^{-1} & A \\ A^T & 0 \end{bmatrix} = \left[ \begin{array}{cc|cc} c_1^{-1} & & -1 & 0 \\ & c_2^{-1} & 1 & -1 \\ \hline -1 & 1 & & \\ 0 & -1 & & \end{array} \right]$$

With  $C = I$  elimination leads to

$$\begin{bmatrix} I & A \\ 0 & -A^T A \end{bmatrix} \quad \text{with} \quad -A^T A = - \begin{bmatrix} 2 & -1 \\ -1 & 1 \end{bmatrix}.$$

The equation...