Statistics 210B, Spring 1998

Class Notes

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Seventh Set of Notes

1   Optimization

For references, see D.G. Luenberger (1969) *Optimization by Vector Space Methods*, John
Wiley and Sons, Inc., NY.; E.J. Anderson and P. Nash, 1987, *Linear Programming in
Infinite-Dimensional Spaces*, Wiley, NY; M.S. Bazaraa and C.M. Shetty, 1979, *Nonlinear
Programming: Theory and Algorithms*, Wiley, NY; Shor, 1985, *Minimization Methods for
Non-Differentiable Functions*, Springer-Verlag, NY.

Many questions in statistical theory can be reduced to optimization problems, sometimes
in infinite-dimensional spaces (spaces of functions or measures, for example). For example,
we have just seen in Donoho's work how the difficulty of certain minimax estimation problems
can be related to the modulus of continuity, whose computation is an optimization problem
over a convex subset of ℓ_2.

Some unconstrained optimization problems with differentiable, convex objective func-
tions, are fairly straightforward to solve, *e.g.*, using the calculus of variations.   Solving
differentiable, unconstrained, convex problems numerically is not typically difficult (descent

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algorithms can be used), unless evaluating the objective functional or its derivative is extremely computationally intensive.

Constrained problems, nondifferentiable problems, and nonconvex problems are typically much harder. Even for convex functions whose derivative exists almost everywhere, the steepest descent algorithm can converge to a nonstationary point (see Shor, Ch. 2, §2.1 for an example). Nondifferentiable objective functionals arise fairly frequently in statistics. For example, the absolute value function is not differentiable at zero, so the problem of finding the median as the solution of the optimization problem of minimizing the sum of the absolute deviations (or of finding a multivariate generalization of the median) is a convex, nondifferentiable optimization problem. Similarly, the objective functionals for minimum ℓ_1 and minimum ℓ_∞ regression are nondifferentiable.

Some quite interesting statistical problems have convex objective functionals, but nonconvex constraints, such as signal recovery problems subject to constraints on the measure of the support of the signal (sparsity constraints).

Linear equality constraints (such as $\langle x, g \rangle = 0$) are fairly straightforward to deal with; one can project the problem onto the subspace where the constraint is satisfied. Linear inequalities are somewhat harder. Two of the most useful tools for solving constrained infinite-dimensional optimization problems are Fenchel and Lagrange duality.

A *cone* in a real linear vector space $\mathcal{X}$ is a set $P \subset \mathcal{X}$ such that if $x \in P$, then $\alpha x \in P$ for all $\alpha > 0$. One can establish a partial order on a vector space $\mathcal{X}$ with a convex cone P (then called the *positive cone*) by defining $x \geq y$ if $x - y \in P$. If $\mathcal{X}$ is a topological space (such as a normed space with topology inherited from the norm), and if the interior of the positive cone P is nonempty in the topology of $\mathcal{X}$, we write $x > y$ if $x - y \in P^\circ$, the interior of P. (Note that this differs from the definition of $<$ we used for a totally ordered set, where $<$ meant $\leq$ but not $=$; here, $<$ derives from topological properties of the positive cone that defines the order.)

If $\mathcal{X}$ is a linear vector space, $\mathcal{X}^*$ denotes the linear space of all linear functionals defined on $\mathcal{X}$, and is called the algebraic dual space of $\mathcal{X}$. If $\mathcal{X}$ is a normed space, by default $\mathcal{X}^*$ is the space of *bounded* linear functionals on $\mathcal{X}$, (called the normed dual space of $\mathcal{X}$) unless otherwise specified. Denote by $\langle x^*, x \rangle$ the action of the linear functional $x^* \in \mathcal{X}^*$ on the

element $x \in \mathcal{X}$. The natural mapping from a space $\mathcal{X}$ to its second dual $\mathcal{X}^{**}$ (the dual of its dual) is $\langle x^{**}, x^* \rangle = \langle x^*, x \rangle$. Clearly each $x \in \mathcal{X}$ gives a linear functional x^{**} on $\mathcal{X}^*$ this way. If every (bounded) linear functional on $\mathcal{X}^*$ can be obtained this way (*i.e.*, if $\mathcal{X}^{**} = \mathcal{X}$), $\mathcal{X}$ is said to be *reflexive*.

The epigraph of a functional f on a set $C \subset \mathcal{X}$ is

$$[f, C]_+ \equiv \{(t, x) \in \mathbf{R} \times \mathcal{X} : x \in C, \ f(x) \le t\}. \tag{1}$$

If C is convex, $[f, C]_+$ is a convex set in $\mathbf{R} \times \mathcal{X}$ iff f is a convex functional. Similarly, let

$$[g, D]_- \equiv \{(t, x) \in \mathbf{R} \times \mathcal{X} : x \in D, \ f(x) \ge r\}. \tag{2}$$

Definition. A *linear variety* in a vector space $\mathcal{X}$ is the translation of a subspace S in $\mathcal{X}$. That is, if S is a subspace, then for every $x \in \mathcal{X}$, $S + x$ is a linear variety. A *hyperplane* H in a vector space $\mathcal{X}$ is a maximal proper linear variety; that is, a linear variety such that if Y is another linear variety in $\mathcal{X}$ and $H \subset Y$, then either $Y = H$ or $Y = X$. A hyperplane can be characterized by a linear functional: every hyperplane can be written as $\{x \in \mathcal{X} : \langle x^*, x \rangle + b = 0\}$ for some $x^* \in \mathcal{X}^*$ and some $b \in \mathbf{R}$. Every set of the form $\{x \in \mathcal{X} : \langle x^*, x \rangle + b = 0\}$ is a hyperplane. If x^* is a nonzero linear functional on a normed vector space $\mathcal{X}$, the hyperplanes $\{x : \langle x^*, x \rangle + b = 0\}$ are closed for every $b \in \mathbf{R}$ iff x^* is continuous.

Theorem 1 *Separating hyperplane theorem. Suppose that C, D are convex subsets of a normed vector space $\mathcal{X}$, that C contains interior points, and that D contains no interior point of C. Then there is a a hyperplane separating the sets: there is an element $x^* \in \mathcal{X}^*$ s.t.*

$$\sup_{x \in C} \langle x^*, x \rangle \le \inf_{x \in D} \langle x^*, x \rangle. \tag{3}$$

Thus there is a number $b \in \mathbf{R}$ s.t.

$$\langle x^*, x \rangle + b \le 0 \qquad \forall x \in C$$
$$\langle x^*, x \rangle + b \ge 0 \qquad \forall x \in D$$

$$\tag{4}$$

1.1 Algebraic Duality

We always take $\inf_{x \in \emptyset} f(x) = \infty$ and $\sup_{x \in \emptyset} f(x) = -\infty$.

For any functional f on a real linear vector space $\mathcal{X}$ with dual $\mathcal{X}^*$ and any sets $C, D \subset \mathcal{X}$ consider the *value of the primal problem*

$$v(\mathcal{P}) \equiv \inf_{x \in C \cap D} f(x). \tag{5}$$

Clearly, for any $x^* \in \mathcal{X}^*$,

$$
\begin{aligned}
v(\mathcal{P}) &= \inf_{x \in C \cap D} \{ f(x) - \langle x^*, x \rangle + \langle x^*, x \rangle \} \\
&\geq \inf_{x \in C \cap D} \langle x^*, x \rangle + \inf_{x \in C \cap D} \{ f(x) - \langle x^*, x \rangle \} \\
&\geq \inf_{x \in D} \langle x^*, x \rangle + \inf_{x \in C} \{ f(x) - \langle x^*, x \rangle \}
\end{aligned}
\tag{6}
$$

This is true for all x^*, so

$$
\begin{aligned}
\inf_{x \in C \cap D} f(x) &\geq \sup_{x^* \in \mathcal{X}^*} \left\{ \inf_{x \in D} \langle x^*, x \rangle + \inf_{x \in C} \{ f(x) - \langle x^*, x \rangle \} \right\} \\
&= \sup_{x^* \in \mathcal{X}^*} \{ D^*[x^*] + C^*[x^*] \},
\end{aligned}
\tag{7}
$$

where

$$C^*[x^*] \equiv \inf_{x \in C} \{ f(x) - \langle x^*, x \rangle \} \tag{8}$$

and

$$D^*[x^*] \equiv \inf_{x \in D} \{ \langle x^*, x \rangle \}. \tag{9}$$

The only functionals x^* it is worth considering are those for which C^* and D^* are greater than $-\infty$. Let

$$C^* \equiv \left\{ x^* \in \mathcal{X}^* : \inf_{x \in C} \{ f(x) - \langle x^*, x \rangle \} > -\infty \right\}, \tag{10}$$

and

$$\mathcal{D}^* \equiv \left\{ x^* \in \mathcal{X}^* : \inf_{x \in D} \langle x^*, x \rangle > -\infty \right\}. \tag{11}$$

Then wlog we can restrict attention to

$$\sup_{x^* \in \mathcal{C}^* \cap \mathcal{D}^*} \{ D^*[x^*] + C^*[x^*] \}, \tag{12}$$

with the supremum defined to be $-\infty$ if $\mathcal{C}^* \cap \mathcal{D}^* = \emptyset$.

In general, the sup over $\mathcal{X}^*$ need not equal the inf over $\mathcal{X}$. When it does not, there is said to be a "duality gap."

Example. Suppose $\mathcal{X}$ is a linear vector space of functions $x = x(t)$ on some fixed domain; $\{x_j^*\}_{j=1}^n \subset \mathcal{X}^*$, $\{x_j^*\}$ linearly independent; $d : \mathcal{X} \to \mathbf{R}^n$, $x \to (\langle x_j^*, x \rangle)_{j=1}^n$; $\Xi \subset \mathbf{R}^n$ is a bounded subset of $\mathbf{R}^n$, $D = \{x \in \mathcal{X} : d(x) \in \Xi\}$. Then one can show that $\mathcal{D}^* = \text{span}\{x_j^*\}_{j=1}^n$ (D is a hypercylinder constrained only in the directions "aligned" with an x_j^*; in other directions D is unconstrained, so a linear functional with a component in any direction not in $\text{span}\{x_j^*\}_{j=1}^n$ is unbounded below on D). Thus for any f and C, the infinite-dimensional problem

$$\inf_{x \in C \cap D} f(x) \tag{13}$$

is bounded from below by a finite-dimensional problem on $\text{span}\{x_j^*\}_{j=1}^n$. For particular sets Ξ and C, and particular functionals f, this can lead to an easy solution for $v(\mathcal{P})$. Continuing the example, suppose that $C = \mathcal{X}$, that $f(x) = \langle x_0^*, x \rangle$, and that

$$\Xi \equiv \{\gamma \in \mathbf{R}^n : \|\gamma - \delta\| \leq \epsilon\}, \tag{14}$$

for some fixed $\delta \in \mathbf{R}^n$ (an ϵ-ball in $\mathbf{R}^n$ centered at δ). Then $\mathcal{C}^* = x_0^*$, and we already saw that $\mathcal{D}^* = \text{span}\{x_j^*\}_{j=1}^n$, so $\mathcal{C}^* \cap \mathcal{D}^* = \emptyset$ unless $x_0^* = \sum_{j=1}^n \alpha_j x_j^*$ for some sequence of constants $\alpha = (\alpha_j)_{j=1}^n$. Given a linearly independent set $\{x_j^*\}_{j=1}^n \subset \mathcal{X}^*$, one can construct a linearly independent set $\{x_j\}_{j=1}^n \subset \mathcal{X}$ such that

$$\langle x_j^*, x_k \rangle = 1_{j=k}. \tag{15}$$

If indeed $x_0^* = \sum_{j=1}^n \alpha_j x_j^*$, then for $x^* \in \mathcal{C}^* \cap \mathcal{D}^*$

$$\inf_{x \in C} \langle x_0^*, x \rangle - \langle x^*, x \rangle = 0. \tag{16}$$

For any $x \in D$, $d(x) = \delta + \nu$ with $\|\nu\| \leq \epsilon$, so for $x \in D$,

$$
\begin{aligned}
\alpha \cdot d(x) &= \alpha \cdot \delta + \alpha \cdot \nu \\
&\geq \alpha \cdot \delta - |\alpha \cdot \nu| \\
&\geq \alpha \cdot \delta - \|\alpha\|\|\nu\| \\
&\geq \alpha \cdot \delta - \epsilon\|\alpha\|. \tag{17}
\end{aligned}
$$

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This bound is in fact attained by setting

$$\beta = \delta - \epsilon \frac{\alpha}{\|\alpha\|} \tag{18}$$

and taking $x = \sum_j \beta_j x_j$. Thus

$$\inf_{x \in D} \langle x^*, x \rangle = \alpha \cdot \delta - \epsilon \|\alpha\|. \tag{19}$$

This gives us

$$\inf_{x \in C \cap D} \langle x_0^*, x \rangle = \begin{cases} \alpha \cdot \delta - \epsilon \|\alpha\|, & x_0^* = \sum_{j=1}^n \alpha_j x_j^* \\ -\infty, & \text{otherwise} \end{cases} \tag{20}$$

There is no duality gap in this problem.

See Stark (1992) *J. Geophys. Res.*, *97*, 14,055–14,082, for more examples.

1.2 Fenchel Duality

Fenchel duality establishes conditions under which there is no duality gap in the algebraic duality relation given in the previous section. The conditions rely on topological considerations, and the version presented here assumes that the spaces are normed, the sets are convex, *etc.* Note that the definitions are changed a bit from the last section!

Let $\mathcal{X}$ be a normed linear vector space with normed dual space $\mathcal{X}^*$, and let C and D be convex subsets of $\mathcal{X}$. Let $f : \mathcal{X} \to \mathbf{R}$ be convex, and let $g : \mathcal{X} \to \mathbf{R}$ be concave. The *conjugate set* $\mathcal{C}^*$ of C is

$$\mathcal{C}^* \equiv \{x^* \in \mathcal{X}^* : \sup_{x \in C}[\langle x^*, x \rangle - f(x)] < \infty\}. \tag{21}$$

The conjugate functional f^* of f is defined on C^* by

$$f^*(x^*) = \sup_{x \in C}[\langle x^*, x \rangle - f(x)]. \tag{22}$$

The *conjugate set* $\mathcal{D}^*$ of D is

$$\mathcal{D}^* \equiv \{x^* \in \mathcal{X}^* : \inf_{x \in D}[\langle x^*, x \rangle - g(x)] > -\infty\}. \tag{23}$$

The conjugate functional g^* of g is defined on D^* by

$$g^*(x^*) = \inf_{x \in D}[\langle x^*, x \rangle - g(x)]. \tag{24}$$

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One may show that $\mathcal{C}^*$ and $\mathcal{D}^*$ are convex subsets of X^*, that f^* is a convex functional, and that g^* is a concave functional.

Theorem 2 *Fenchel Duality (see Luenberger, 1969, §7.12, Theorem 1). Let $\mathcal{X}$ be a normed space, C and D be convex subsets of $\mathcal{X}$, f a convex functional on $\mathcal{X}$, g a concave functional on $\mathcal{X}$. Suppose $C \cap D$ contains points in the relative interior of C and D, and that either $[f, C]_+$ or $[g, D]_-$ has nonempty interior. If*

$$v(\mathcal{P}) = \inf_{x \in C \cap D}\{f(x) - g(x)\} > -\infty, \tag{25}$$

then

$$v(\mathcal{P}) = \max_{x^* \in C^* \cap D^*}\{g^*(x^*) - f^*(x^*)\}. \tag{26}$$

The max on the right is attained by some $x_0^* \in C^* \cap D^*$. If the infimum is attained by some $x_0 \in C \cap D$, then

$$\max_{x \in C}[\langle x_0^*, x \rangle - f(x)] = \langle x_0^*, x_0 \rangle - f(x_0) \tag{27}$$

and

$$\min_{x \in D}[\langle x_0^*, x \rangle - g(x)] = \langle x_0^*, x_0 \rangle - g(x_0). \tag{28}$$

Remark. I cannot see where in the proof of the Fenchel Duality theorem Luenberger uses the hypothesis that $C \cap D$ contains points in the relative interior of C and D. Furthermore, that hypothesis is not necessarily satisfied in the example he gives to the min-max theorem of games—see below (a compact convex subset of a reflexive space does not necessarily have nonempty interior). Thanks to Jason Schweinsberg and Von Bing Yap for pointing out these problems! Can anyone see how the hypothesis enters the proof?

Example. The min-max theorem in game theory. Let $\mathcal{X}$ be a normed linear vector space and $\mathcal{X}^*$ its normed dual. Assume $\mathcal{X}$ is reflexive. Player A selects a strategy x from $\mathcal{A} \subset \mathcal{X}$ and player B selects a strategy from $\mathcal{B}^* \subset \mathcal{X}^*$, without knowledge of player A's choice. Player A pays player B $\langle x^*, x \rangle$. Player A thus wants to minimize $\langle x^*, x \rangle$, while player B wants to maximize it. Suppose both players seek a minimax strategy: one in which they lose least (gain most) in the worst case. Thus player A seeks

$$v_- = \inf_{x \in \mathcal{A}} \sup_{x^* \in \mathcal{B}^*} \langle x^*, x \rangle, \tag{29}$$

while player B seeks

$$v_+ = \sup_{x^* \in \mathcal{B}^*} \inf_{x \in \mathcal{A}} \langle x^*, x \rangle. \tag{30}$$

Theorem 3 *(Min-max theorem; see Luenberger, §7.13, Theorem 1.) Suppose $\mathcal{A}$ and $\mathcal{B}^*$ are compact and convex. Then*

$$\inf_{x \in \mathcal{A}} \sup_{x^* \in \mathcal{B}^*} \langle x^*, x \rangle = \sup_{x^* \in \mathcal{B}^*} \inf_{x \in \mathcal{A}} \langle x^*, x \rangle. \tag{31}$$

Proof. Define

$$
\begin{aligned}
f : \mathcal{X} &\rightarrow \mathbf{R} \\
x &\mapsto \max_{x^* \in \mathcal{B}^*} \langle x^*, x \rangle.
\end{aligned} \tag{32}
$$

The max is attined because $\mathcal{B}^*$ is compact (by assumption) and x, viewed as an element of $\mathcal{X}^{**}$, is a continuous function on $\mathcal{B}^*$. By linearity and the convexity of $\mathcal{B}^*$, for all $\alpha \in [0, 1]$,

$$
\begin{aligned}
f(\alpha x + (1 - \alpha) y) &= \max_{x^* \in \mathcal{B}^*} \langle x^*, \alpha x + (1 - \alpha) y \rangle \\
&= \max_{x^* \in \mathcal{B}^*} [\langle x^*, \alpha x \rangle + \langle x^*, (1 - \alpha) y \rangle] \\
&= \max_{x^* \in \mathcal{B}^*} [\alpha \langle x^*, x \rangle + (1 - \alpha) \langle x^*, y \rangle] \\
&\leq \max_{x^* \in \mathcal{B}^*} \alpha \langle x^*, x \rangle + \max_{x^* \in \mathcal{B}^*} (1 - \alpha) \langle x^*, y \rangle \\
&= \alpha f(x) + (1 - \alpha) f(y).
\end{aligned} \tag{33}
$$

Assignment. Show that f is continuous, and that there exist points in the $C \cap D$ in the relative interior of C and D.

We seek $\min_{x \in \mathcal{A}} f(x)$. Apply Fenchel duality, identifying C with $\mathcal{X}$, $g = 0$, and D with $\mathcal{A}$. Because D is a compact set, $\mathcal{D}^* = \mathcal{X}^*$, and

$$g^*(x^*) = \min_{x \in \mathcal{A}} \langle x^*, x \rangle. \tag{34}$$

Consider $\mathcal{C}^*$. Suppose $x_1^* \notin \mathcal{B}^*$. Then (by the separating hyperplane theorem) there exists $x_1 \in \mathcal{X}$ and $\alpha \in \mathbf{R}$ such that

$$\langle x_1^*, x_1 \rangle - \langle x^*, x_1 \rangle > \alpha > 0, \quad \forall x^* \in \mathcal{B}^*. \tag{35}$$

Thus letting $x = ax_1$ with $a > 0$ sufficiently large,

$$\langle x_1^*, x \rangle - \max_{x^* \in \mathcal{B}^*} \langle x^*, x \rangle = \langle x_1^*, x \rangle - f(x) \tag{36}$$

can be made arbitrarily large, so $x_1^* \notin \mathcal{C}^*$. On the other hand, if $x_1^* \in \mathcal{B}^*$,

$$\sup_{x \in \mathcal{X}} \langle x_1^*, x \rangle - \max_{x^* \in \mathcal{B}^*} \langle x^*, x \rangle = 0, \tag{37}$$

and is attained by $x = 0$. Thus $\mathcal{C}^* = \mathcal{B}^*$. The conditions of Fenchel duality apply, and hence

$$\min_{x \in \mathcal{A}} f(x) = \max_{x^* \in \mathcal{B}^* \cap \mathcal{X}^*} g^*(x^*) = \max_{x^* \in \mathcal{B}^*} \min_{x \in \mathcal{A}} \langle x^*, x \rangle. \tag{38}$$

Example (of something): Seminorm minimization in a Hilbert Space, and Splines.

Regularized least squares is an estimator sometimes used in nonparametric regression. The idea is to find the regression function of minimum Sobolev norm (a norm that involves derivatives of the function) among those that fit the data within an ℓ_2 tolerance, or (equivalently) to find the model that fits the data best in an ℓ_2 sense among those whose Sobolev norm does not exceed some bound.

Recall that a real inner-product space is a real linear vector space $\mathcal{X}$ with an additional operation $\langle \cdot, \cdot \rangle : \mathcal{X} \times \mathcal{X} \to \mathbf{R}$ with the properties that for all $x, y, z \in \mathcal{X}$ and all $\gamma \in \mathbf{R}$,

$$
\begin{aligned}
\langle x, y \rangle &= \langle y, x \rangle \\
\langle x + y, z \rangle &= \langle x, z \rangle + \langle y, z \rangle \\
\langle \gamma x, y \rangle &= \gamma \langle x, y \rangle \\
\langle x, x \rangle &\geq 0 \\
\langle x, x \rangle = 0 &\Rightarrow x = 0
\end{aligned}
\tag{39}
$$

The functional $\|x\| \equiv \sqrt{\langle x, x \rangle}$ is a norm on a (real) inner-product space. A real inner-product space that is complete in the norm topology (*i.e.*, in which all Cauchy sequences have limits in the space) is called a Hilbert space. Hilbert spaces are their own normed dual spaces. A normed vector space $\mathcal{X}$ is *separable* if there is a countable set $\{x_j\}_{j=1}^{\infty}$ such that every element $x \in \mathcal{X}$ can be approximated arbitrarily well (in the norm) by a finite linear combination of $\{x_j\}_{j=1}^{\infty}$. All separable Hilbert spaces are isomorphic to ℓ_2. Every real inner product space

can be "completed" to form a Hilbert space by considering elements to be equivalence classes of Cauchy sequences.

For any x, y in an inner-product space $\mathcal{X}$, $|\langle x, y \rangle| \leq \|x\| \cdot \|y\|$. Two elements x and y in an inner-product space are said to be *orthogonal* if $\langle x, y \rangle = 0$; then we write $x \perp y$. If $x \perp y$ then $\|x + y\|^2 = \|x\|^2 + \|y\|^2$. An element x of an inner product space is orthogonal to a subset M of the same inner product space if $x \perp y \ \forall y \in M$; then we write $x \perp M$. Two subsets M, N of an inner product space are orthogonal if $x \perp y \ \forall x \in M$ and $\forall y \in N$; then we write $M \perp N$. The *orthogonal complement* of a set $M \subset \mathcal{X}$ is

$$M^\perp = \{x \in \mathcal{X} : x \perp M\}. \tag{40}$$

For any $M \subset \mathcal{X}$, $M^\perp$ is a closed subspace. If M is a closed subspace of $\mathcal{X}$, each $x \in \mathcal{X}$ has a unique decomposition $x = m + n$ where $m \in M$ and $n \in M^\perp$; we write $\mathcal{X} = M \oplus M^\perp$. Every finite-dimensional subspace of a Hilbert space is closed.

Lemma 1 *Let $\{x_j\}_{j=1}^n \subset \mathcal{X}$ be a linearly independent set, $M = \mathrm{span}\{x_j\}_{j=1}^n$, and $\delta \in \mathbf{R}^n$. Then*

$$\arg \min_{x \in \mathcal{X}} \{\|x\| : \langle x_j, x \rangle = \delta_j, \ \ j = 1, \cdots, n\} \in M. \tag{41}$$

The minimum is attained, and by a unique element of M.

Proof. M is a closed subspace of $\mathcal{X}$, so we can decompose every x into a sum $x = x_M + x_{M^\perp}$ with $x_M \in M$ and $x_{M^\perp} \in M^\perp$, and $\|x\|^2 = \|x_M\|^2 + \|x_{M^\perp}\|^2$. Now $\langle x_j, x_{M^\perp} \rangle = 0$ for all j, so $\langle x_j, x \rangle = \langle x_j, x_M \rangle$. Thus if $\langle x_j, x \rangle = \delta_j \ \forall j$, then $\langle x_j, x_M \rangle = \delta_j \ \forall j$, but $\|x\| \geq \|x_M\|$. Thus it suffices to consider $x \in M$. Because $\{x_j\}_{j=1}^n$ is a linearly independent set, there is a unique vector $x_0 \in M$ s.t. $\langle x_j, x_0 \rangle = \delta_j$. Even if $\{x_j\}$ were not linearly independent, that the minimum is attained would follow from the fact that M is a closed subspace of $\mathcal{X}$, and therefore complete. Any sequence of elements of M for which the norm converges to the minimal value can be shown to be a Cauchy sequence within M, so its limit is in M. The uniqueness would then follow from the strict convexity of the norm in Hilbert space.

Remark. Essentially the same proof shows that if M is a closed subspace and $x \in \mathcal{X}$,

$$\min_{m \in M} \|x - m\| \tag{42}$$

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is attained by an element m_0 of M, and that $x - m_0 \in M^\perp$.

Remark. Let $\langle \mathbf{x}, x \rangle = (\langle x_j, x \rangle)_{j=1}^n$. It follows from Lemma 1 that if $\Xi \subset \mathbf{R}^n$, and x_0 solves

$$\min\{\|x\| : \langle \mathbf{x}, x \rangle \in \Xi\}, \tag{43}$$

then $x_0 \in M = \operatorname{span}\{x_j\}_{j=1}^n$.

Let S be a closed subspace of $\mathcal{X}$. Then

$$|x|_S = \min_{s \in S} \|x - s\| \tag{44}$$

is a seminorm.

Assignment. Verify that for a closed subspace S of a Hilbert space $\mathcal{X}$, $|\cdot|_S$ is a seminorm.

Let $S = \operatorname{span}\{s_k\}_{k=1}^m$ be a finite-dimensional (and therefore closed) subspace of $\mathcal{X}$. Consider the problem of finding

$$\min\{|x|_S : \langle \mathbf{x}, x \rangle = \delta\}, \tag{45}$$

with $\{x_j\}_{j=1}^n$ linearly independent. Any x can be decomposed into $x_S + x_{S^\perp}$, with $x_S \in S$ and $x_{S^\perp} \in S^\perp$. Let $\langle \mathbf{x}, S \rangle = \{\langle \mathbf{x}, s \rangle : s \in S\}$. Taking $\Xi = \delta + \langle \mathbf{x}, S \rangle$, the problem becomes

$$\min\{\|x\| : \langle \mathbf{x}, x \rangle \in \Xi\}. \tag{46}$$

The optimal x_0 is thus a linear combination of $\{x_j\}_{j=1}^n$, plus an element of S; we restrict attention to the subspace of $\mathcal{X}$ consisting of linear combinations of elements of S and $\{x_j\}_{j=1}^n$. Define Γ to be the n by n matrix with elements $\Gamma_{ij} = \langle x_i, x_j \rangle$. Because $\{x_j\}$ is linearly independent and $\langle \cdot, \cdot \rangle$ is symmetric, Γ is a positive-definite symmetric matrix. Let Λ be the n by m matrix with elements $\Lambda_{ij} = \langle x_i, s_j \rangle$. Write

$$x = \gamma \cdot \mathbf{x} + \lambda \cdot \mathbf{s} = \sum_{j=1}^n \gamma_j x_j + \sum_{j=1}^m \lambda_j s_j. \tag{47}$$

The component of x in S does not contribute to $|x|_S$, so $|x|_S^2 \leq \gamma \cdot \Gamma \cdot \gamma$, with equality if $\gamma \cdot \mathbf{x} \perp S$. For the optimal x, that must hold; otherwise, the component could be absorbed into x_S, thereby decreasing $|x|_S$. Thus the seminorm minimization problem is to find

$$\begin{aligned} v(\mathcal{P}) &= \min_{\gamma \in \mathbf{R}^n, \lambda \in \mathbf{R}^m} \{\langle \gamma \cdot \mathbf{x}, \gamma \cdot \mathbf{x} \rangle : \langle \mathbf{x}, \lambda \cdot \mathbf{s} + \gamma \cdot \mathbf{x} \rangle = \delta\} \\ &= \min\{\gamma \cdot \Gamma \cdot \gamma : \Gamma \cdot \gamma + \Lambda \cdot \lambda = \delta\} \end{aligned} \tag{48}$$

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As just argued, for the optimal x, $\langle s_j, \gamma \cdot \mathbf{x} \rangle = 0$, $j = 1, \cdots, m$, so $\Lambda^T \cdot \gamma = 0$. This gives the coefficients of x through solving

$$
\begin{bmatrix} \Gamma & \Lambda \\ \Lambda^T & 0 \end{bmatrix} \cdot \begin{bmatrix} \gamma \\ \lambda \end{bmatrix} = \begin{bmatrix} \delta \\ 0 \end{bmatrix},
\tag{49}
$$

which has a unique solution if the matrix on the left is nonsingular. That holds if the projections of $\{s_j\}$ onto span$\{x_j\}$ are linearly independent.

This was for the case that $\langle \mathbf{x}, x \rangle = \delta$. If instead we require only $\langle \mathbf{x}, x \rangle \in \Xi$, the same argument shows that the optimal x_0 is a linear combination of $\{x_j\}_{j=1}^n \cup \{s_j\}_{j=1}^m$.

1.3   Quadratic Smoothing Splines

Let $\mathcal{X}$ be the set of functions $x = x(t)$ on the interval $[0, 1]$ that are absolutely continuous, have absolutely continuous first derivatives, and have Lebesgue square-integrable second derivatives. Let $x' = x'(t) = dx/dt$, and $x'' = x''(t) = d^2x/dt^2$. Endow $\mathcal{X}$ with the norm

$$
\|x\|^2 = x^2(0) + |x'(0)|^2 + \int_0^1 (x''(t))^2 \, dt.
\tag{50}
$$

This norm derives from the inner product

$$
\langle x, y \rangle = x(0)y(0) + x'(0)y'(0) + \int_0^1 x''(t)y''(t)dt.
\tag{51}
$$

($I.e.$, $\|x\| = \sqrt{(\langle x, x \rangle)}$.)

Problem. Show that $\mathcal{X}$ is indeed a Hilbert space: verify that $\langle \cdot, \cdot \rangle$ is an inner product, and that $\mathcal{X}$ is complete w.r.t. the induced norm topology.

The space $\mathcal{X}$ is in fact a reproducing kernel Hilbert space (RKHS). A RKHS is a Hilbert space of functions $x = x(t)$ for which the functional that evaluates each function x at the point t_0 (the point-evaluator) is a bounded linear functional; that is, evaluating any x at the point t_0 can be written as the inner product of x with a function $e_{t_0} \in \mathcal{X}$. (Clearly, point-evaluation is linear if the addition of functions and multiplication of functions by scalars is defined in the standard way:

$$
\begin{aligned}
(x + y)(t) &= x(t) + y(t), \quad x, y \in \mathcal{X} \\
(\alpha x)(t) &= \alpha(x(t)), \quad x \in \mathcal{X}, \ \alpha \in \mathbf{R}.
\end{aligned}
$$

The issue is whether this linear functional is bounded.) In the present case,

$$
\begin{aligned}
x(t_0) &= x(0) + x'(0)t_0 + \int_0^{t_0} du \int_0^u ds x''(s) \\
&= x(0) + x'(0)t_0 + \int_0^1 du 1_{u \leq t_0} \int_0^1 ds x''(s) 1_{s \leq u} \\
&= x(0) + x'(0)t_0 + \int_0^1 ds x''(s) \int_0^1 du 1_{u \leq t_0} 1_{u \geq s} \\
&= x(0) + x'(0)t_0 + \int_0^1 ds x''(s)(t_0 - s)_+.
\end{aligned}
\tag{52}
$$

Formally, this looks like the inner product with an element $e_{t_0} \in \mathcal{X}$ whose value at 0 is 1, whose derivative at 0 is t_0, and whose second derivative is $e''_{t_0}(t) = (t_0 - t)_+$. The question is whether $e(t) \in \mathcal{X}$. It is: it is absolutely continuous and has absolutely continuous first derivative, and bounded second derivative, so its $\mathcal{X}$-norm is finite. We have

$$
e_{t_0}(t) = \begin{cases} 1 + t_0 t + t_0 \frac{t^2}{2} - \frac{t^3}{6} & t \leq t_0 \\ 1 + t_0 t + t \frac{t_0^2}{2} - \frac{t_0^3}{6} & t > t_0. \end{cases}
\tag{53}
$$

For any collection of distinct points $\{t_j\}_{j=1}^n$, the set of functions $\{e_{t_j}\}_{j=1}^n \subset \mathcal{X}$ is linearly independent.

Define the seminorm $|x|$ for $x \in \mathcal{X}$ by

$$
|x|^2 = \int_0^1 (x''(t))^2 \, dt.
\tag{54}
$$

Let $S = \mathrm{span}\{1, t\}$. Then $S^\perp \equiv \{x \in \mathcal{X} : x(0) = x'(0) = 0\}$. The seminorm $|\cdot|$ can be viewed as the square of the norm of the orthogonal projection $P_{S^\perp}$ of x onto the (closed) subspace $S^\perp$; i.e.,

$$
|x| = \|P_{S^\perp} x\| = \inf_{\ell \in S} \|x - \ell\| = \|x - P_S x\|.
\tag{55}
$$

This is a continuous functional on $\mathcal{X}$: consider a sequence $x_k \to x$ in the norm. The operator norm of a Hilbert-space projection is unity; that is, for any subspace $M \subset \mathcal{X}$, $\|P_M x\| \leq 1 \times \|x\|$. By the triangle inequality, $\|x + (y - x)\| \leq \|x\| + \|y - x\|$, and $\|y + (x - y)\| \leq \|y + \|x - y\|$; together these imply that $\|\|x\| - \|y\|\| \leq \|x - y\|$. Thus

$$
\begin{aligned}
\|\|P_{S^\perp} x_k\| - \|P_{S^\perp} x_j\|\| &\leq \|P_{S^\perp} x_k - P_{S^\perp} x_j\| \\
&= \|P_{S^\perp}(x_k - x_j)\| \\
\leq \|x_k - x_j\| &\to 0
\end{aligned}
\tag{56}
$$

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Now S is finite dimensional, and therefore closed, so we have $\mathcal{X} = S \oplus S^\perp$. For any $x \in \mathcal{X}$, let $x_S + x_{S^\perp}$ be the (unique) decomposition of x into its components $x_S \in S$ and $x_{S^\perp} \in S^\perp$. Then $|x| = \|x_{S^\perp}\|$. Let $e_j = e_{t_j}$, $j = 1, \cdots, n$. Let $\langle \mathbf{e}, x \rangle = (\langle e_j, x \rangle)_{j=1}^n$. Because each e_j is a continuous linear functional on $\mathcal{X}$ and the two-norm on $\mathbf{R}^n$ is continuous, for any $\delta \in \mathbf{R}^n$ and any $\epsilon > 0$,

$$D \equiv \{ x \in \mathcal{X} : \| \langle \mathbf{e}, x \rangle - \delta \| \le \epsilon \} \tag{57}$$

is a closed convex subset of $\mathcal{X}$. The smoothing spline optimization problem is to find a function x_0 that attains $v(\mathcal{P})$,

$$v(\mathcal{P}) \equiv \inf_{x \in D} |x|, \tag{58}$$

which is a seminorm minimization problem of the type just explored. It follows that $v(\mathcal{P})$ is attained, and the optimal vector x_0 is a linear combination of 1, t, and $\{e_j\}_{j=1}^n$. That is, x_0 is an absolutely continuous piecewise cubic function with absolutely continuous first derivative and square-integrable second derivative.

To try to add some intuition, consider what the solution would be like were $\{e_j\}_{j=1}^n \perp S$. Then there would be no advantage to including an element of S in the solution, and the optimal x_0 would just be a linear combination of $\{e_j\}$. However, if the subspace spanned by $\{e_j\}$ is not orthogonal to S, a part of the data can be produced by an element of S. The left over part of the data can still be produced using just a linear combination of $\{e_j\}$, and there is no advantage to going outside the subspace spanned by $S \cup \{e_j\}$. Define $\Gamma_{ij} = \langle e_i, e_j \rangle$ and $\Lambda_{ij} = \langle e_i, s_j \rangle$. The seminorm ignores any component of S remaining in the "extra" linear combination of $\{e_j\}$, so the optimal solution is of the form $x_0 = x_{0S} + x_{0S^\perp}$, where $x_{0S^\perp} = \alpha \cdot \mathbf{e}$ with $\Lambda \cdot \alpha = 0$.

We can also apply Fenchel duality to this problem. Let $f(x) = |x|_S^2$, $C = \mathcal{X}$, and $g(x) = 0$. Because $\{e_j\}$ is a linearly independent subset of $\mathcal{X}$ and f is continuous, provided $\epsilon > 0$, the epigraph $[f, D]_+$ has nonempty relative interior. The conjugate set $\mathcal{C}^*$ of C is

$$
\begin{aligned}
\mathcal{C}^* & \equiv \{ x^* \in \mathcal{X}^* : \sup_{x \in C} [\langle x^*, x \rangle - f(x)] < \infty \} \\
& = \{ x \in \mathcal{X} : \sup_{y \in \mathcal{X}} [\langle x, y \rangle - |y|] < \infty \} \\
& = S^\perp \cap B(1),
\end{aligned}
\tag{59}
$$

where $B(1) = \{x \in \mathcal{X} : \|x\| \leq 1\}$. The dual functional of f is

$$
\begin{aligned}
f^*(x^*) &= \sup_{x \in C}[\langle x^*, x \rangle - f(x)] \\
&= \sup_{x \in \mathcal{X}}[\langle x^*, x \rangle - |x|_S^2] \\
&= \begin{cases} 0, & x^* \in S^\perp \cap B(1) \\ \infty, & \text{otherwise}, \end{cases}
\end{aligned}
\tag{60}
$$

The conjugate set $\mathcal{D}^*$ of D is

$$
\begin{aligned}
\mathcal{D}^* &\equiv \{x \in \mathcal{X} : \inf_{y \in D}[\langle x, y \rangle - g(y)] > -\infty\} \\
&= \{x \in \mathcal{X} : \inf_{y \in D}[\langle x, y \rangle] > -\infty\} \\
&= \operatorname{span}\{e_j\}_{j=1}^n.
\end{aligned}
\tag{61}
$$

The conjugate functional g^* of g is

$$
\begin{aligned}
g^*(x^*) &= \inf_{x \in D}[\langle x^*, x \rangle - g(x)] \\
&= \begin{cases} -\infty, & x^* \notin \operatorname{span}\{e_j\}_{j=1}^n \\ \alpha \cdot \delta - \epsilon \|\alpha\|, & x^* = \sum_j \alpha_j e_j, \end{cases}
\end{aligned}
\tag{62}
$$

on substituting the result we obtained in the section on algebraic duality. This leads to the dual problem

$$
v(\mathcal{D}) = \max_{\alpha \in \mathbf{R}^n : \sum_j \alpha_j e_j \perp S; \|\alpha \cdot \mathbf{e}\| \leq 1} \{\alpha \cdot \delta - \epsilon \|\alpha\|\}.
\tag{63}
$$

Taking Λ and Γ to be defined as above, this yields

$$
v(\mathcal{D}) = \max_{\alpha \in \mathbf{R}^n : \alpha \cdot \Lambda = 0; \alpha \cdot \Gamma \cdot \alpha \leq 1} \{\alpha \cdot \delta - \epsilon \|\alpha\|\}.
\tag{64}
$$

This maximum is attained by some $x_0^* = \sum_j \alpha_j e_j$. Because the value of the primal problem is also attained by some $x_0 \in \mathcal{X}$, we can use the last part of the Fenchel duality theorem to characterize x_0:

$$
\begin{aligned}
\min_{x \in D} \langle x_0^*, x \rangle &= \alpha \cdot \delta - \epsilon \|\alpha\| \\
&= \langle x_0^*, x_0 \rangle,
\end{aligned}
\tag{65}
$$

and

$$
\max_{x \in C}[\langle x_0^*, x \rangle - |x|] = \langle x_0^*, x_0 \rangle - |x_0| = 0.
\tag{66}
$$

One can use these relations to find x_0 explicitly in terms of α.

1.4   Lagrange Duality

Theorem 4 *(See D.G. Luenberger, 1969.* Optimization by Vector Space Methods, *Wiley, NY., §8.6, Theorem 1.) Let*

$$\mu = \inf\{f(x) : x \in C, \ G(x) \leq 0 \in \mathcal{Z}\}, \tag{67}$$

where C is a convex subset of a linear vector space $\mathcal{X}$, f is a real-valued convex functional on $C \subset \mathcal{X}$, G is a convex mapping from C into a normed space $\mathcal{Z}$ with positive cone P, which is assumed to have non-empty interior. Let $\mathcal{Z}^*$ be the normed dual space of $\mathcal{Z}$ (the space of all bounded linear functionals on $\mathcal{Z}$), and let P^* be the positive cone in $\mathcal{Z}^*$ induced by P (the set of linear functionals $z^* \in \mathcal{Z}^*$ that are nonnegative for all $z \in P$). Suppose that $-\infty < \mu < \infty$, and that $\exists y \in C$ s.t. $G(y) < c$ ($G(y)$ is in the interior of $\theta - P$). For $z^* \in P^*$ define

$$\phi(z^*) \equiv \inf_{x \in C}\{f(x) + \langle z^*, G(x) \rangle. \tag{68}$$

Then

$$\mu = \inf_{G(x) \leq 0, \ x \in C} f(x) = \max_{z^* \geq 0} \phi(z^*) \tag{69}$$

The maximum on the right is attained by some $z_0^* \geq 0$. If the infimum on the left is attained by some $x_0 \in C$, then

$$\langle z_0^*, G(x_0) \rangle = 0, \tag{70}$$

and x_0 maximizes

$$f(x) + \langle z_0^*, G(x) \rangle \tag{71}$$

over all $x \in C$.

Example: Linear Programming Let C be the positive orthant in $\mathbf{R}^n$. Define $\mathcal{Z} = \mathbf{R}^m$, endowed with the supremum norm $\|z\|_\infty = \max_{1 \leq i \leq n} |z_i|$, and the positive cone $P = \{z : z_j \geq 0, \ j = 1, \ldots, m\}$. Note that P has nonempty interior in the sup-norm topology. Let $c \in \mathbf{R}^m$. The dual space of $\mathcal{Z}$ is $\mathcal{Z}^* = \mathbf{R}^m$; its induced positive cone is the usual positive orthant. Let A be an m by n matrix, and let $G(x) = A \cdot x - c$. Let $f(x) = f \cdot x$ for some $f \in \mathbf{R}^n$. We seek

$$\mu = \inf_{x \geq 0 \in \mathbf{R}^n}\{f \cdot x : A \cdot x - c \leq 0\}. \tag{72}$$

This is of the canonical form given.

Suppose there exists $x \geq 0 \in \mathbf{R}^n$ s.t. $A \cdot x < 0$, and that μ is finite. The theorem says that

$$\mu = \max_{y \in \mathbf{R}^m : y \geq 0} \inf_{x \in \mathbf{R}^n : x \geq 0} \{f \cdot x + y \cdot (A \cdot x - c)\}. \tag{73}$$

The infimum is $-\infty$ unless $f + y \cdot A \geq 0$, in which case it is $-y \cdot c$.

The dual problem is thus

$$\max_{y \geq 0 : -A^T \cdot y - f \leq 0} -c \cdot y, \tag{74}$$

which is another linear program.

Example: Quadratic Programming. Let $\Omega = \mathbf{R}^n$, $b \in \mathbf{R}^n$, Q a positive-definite, symmetric n by n matrix, A an m by n matrix, $c \in \mathbf{R}^m$. We seek

$$v(\mathcal{P}) = \min_{x \in \mathbf{R}^n : A \cdot x \leq c} \frac{1}{2} x \cdot Q \cdot x - b \cdot x. \tag{75}$$

This is called a quadratic program. If there exists x s.t. $A \cdot x < c$, then

$$v(\mathcal{P}) = \max_{\lambda \geq 0} \min_x \{\frac{1}{2} x \cdot Q \cdot x - b \cdot x + \lambda \cdot (A \cdot x - c)\}. \tag{76}$$

In this case, the minimization problem is the unconstrained, and is solved by

$$x = Q^{-1}(b - A \cdot \lambda). \tag{77}$$

Let $R = AQ^{-1}A^T$ and $d = c - AQ^{-1}b$. Then

$$v(\mathcal{P}) = \max_{\lambda \geq 0} \left\{ -\frac{1}{2}\lambda \cdot R \cdot \lambda - \lambda \cdot d - \frac{1}{2}b \cdot Q^{-1} \cdot b \right\}, \tag{78}$$

which is another quadratic program. If $m < n$, the new (dual) program can be substantially simpler than the original.