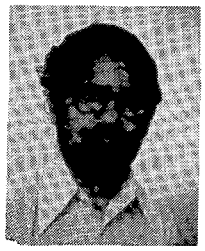

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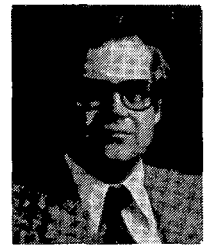

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Stochastic Optimization in System Design

GREGOR KJELLSTRÖM AND LARS TAXÉN

Abstract—**The nonlinear optimization problem and statistical design problem can both be formulated as a region search problem. In this paper, we present a stochastic optimization process, suitable for optimizing functions of a certain measure over generalized regions in R^n. Conditions for an optimal process are discussed, and examples of a wide range of different optimization problems are given. These include the optimization of constrained, discontinuous and random functions in both discrete and continuous variable space. Design centering and tolerancing of large size systems subject to environmental disturbances are also treated.**

I. Introduction

DURING THE LAST decades, optimization has become a basic tool in system design, and a number of highly efficient optimization algorithms have been developed. However, most of these methods assume some inherent property of the objective function to work satisfactorily. For example, in order to utilize gradients or difference quotients, the objective function must be deterministic, i.e., not subject to random variations. Other assumed properties may be linearity or continuity. If the nature of the objective function does not correspond to the algorithm, one usually has to reformulate the original task. Examples of this are the application of iterative linear programming techniques to optimize nonlinear functions [1] or the transformation of a constrained problem into an unconstrained one with the aid of penalty functions [2].

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In this paper we are concerned with the problem of finding an efficient optimization procedure when no particular assumption about the nature of the objective function is made. This problem was posed back in the late 1960's [9], and the result presented here is a followup and further development of earlier works [9], [11], [13], [14], [25].

One reason for posing this problem is of course the possibility of using the same method without modifications on different classes of problems such as constrained or unconstrained ones. Another reason is that it may sometimes be difficult to determine the structure of the objective function, i.e., we have some kind of black-box situation. Thus in real-time computer-aided tuning or optimization, the function value may be affected by noise or measurement errors. Also, computational errors due to limited accuracy may be treated as noise, and if the optimization method can handle this, it can be expected to work better on a computer with small wordlength. Other black-box situations can be found in some biological and psychological experiments, where the objective function can only be evaluated subjectively.

Furthermore, in situations like tolerancing and design centering of toleranced systems, one typically has to evaluate the yield of the system:

$$P = \int_{\mathcal{Q}_0} dV(x) \tag{1.1}$$

where $V(x)$ is the statistical distribution of the system

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elements and $\mathcal{A}_0$ is a region implicitly determined by the specification for the system.

Since it is not possible in general to evaluate (1.1) analytically, various approximate methods have been proposed. Director [3] replaces $\mathcal{A}_0$ with a simplex of interior bounding hyperplanes, and Butler [4] uses a two-dimensional pattern search. Another approach is to constrain P to be equal to 1, which means a worst-case design [5].

These methods work well if the number of elements is small (say less than 10), and the functions defining $\mathcal{A}_0$ are well behaved. However, in practical design tasks, $\mathcal{A}_0$ is usually nonconvex and the complement of $\mathcal{A}_0$ may even be nonconnected [21]. Moreover, it is not unusual to have a large number of elements (of the order of 50 or more). In this case the optimal yield is almost always less than 1, since a worst-case solution is too expensive (it may however serve as a good starting point for the further optimization). The only realistic way to evaluate the integral is then by the means of some Monte Carlo procedure. The estimate for P, say $\hat{P}$, will then be a random variable, since $\hat{P}$ depends on the generated samples. Thus a method assuming deterministic functions cannot be straightforwardly used to optimize a function of $\hat{P}$. In this case, a different approach (such as, e.g., [6], [7], [13], [14], [22]) is to be preferred, where Monte Carlo methods are used not only to evaluate a given design, but also to optimize that design.

In design situations like those above, it turns out that a major problem is to localize and in some sense describe the usually complicated region $\mathcal{A}_0$, defined by the functional mapping from the specification space to the element or component space.

In this paper we investigate the properties of a stochastic search process, which optimizes certain functions of a measure over such regions. The search is done by sampling from a distribution with maximum dispersion, which means that the regions may be of a very complicated nature. This implies that a wide variety of function classes can be optimized. The relevance of this approach is demonstrated by various examples in different applications.

In Section II, the basic concepts are given, and in Section III, optimality conditions for the process are derived. The implementation of the process and some questions concerning convergence are discussed in Sections IV and V, respectively, and finally, application to nonlinear optimization and statistical design (design centering and tolerancing) are treated in Sections VI and VII.

II. Definitions and Assumptions

We begin by making some definitions, suitable for the black-box situation we are interested in. The concepts used here should be considered as convenient labels only, and need not necessarily have any physical meaning.

$\mathcal{Z}$	Specification or output space.
$\mathcal{B} \subset \mathcal{Z}$	Specification in $\mathcal{Z}$ (a subset of $\mathcal{Z}$).
$(\mathcal{X}, \mathcal{Y}) = R^{n+m}$	Component, or input space.
(X, Y)	Random variable of dimension $(n+m)$ and with range in $(\mathcal{X}, \mathcal{Y})$.
$f: (\mathcal{X}, \mathcal{Y}) \to \mathcal{Z}$	Function from $(\mathcal{X}, \mathcal{Y})$ to $\mathcal{Z}$.
$(x, y) \in (\mathcal{X}, \mathcal{Y})$	Realization or sample of (X, Y) in $(\mathcal{X}, \mathcal{Y})$.
$z \in \mathcal{Z}$	Response point in $\mathcal{Z}$, given by $z = f(x, y)$.

The problem we are addressing is to manipulate the black box D, defined by

$$D = \{f, \theta\}, \qquad \theta\text{: designable parameters of } D$$

such that the quality- or objective function

$$C = c(\theta, \mathcal{G}), \qquad C\text{: scalar; } \mathcal{G}\text{: constraint space}$$

is optimized under certain constraints $\mathcal{G}$, which are defined over $\mathcal{B}$ in some way. In doing so, the only property we assume about D is the ability to return a function value $f(x, y)$ for each input sample (x, y).

As designable parameters θ, we will take the parameters (or moments) characterizing the distribution function of X, i.e., we assume that $X = X(\theta)$. The Y distribution is introduced in order to treat the optimization of random functions (Section VI), and we assume that it is known only by sampling and that we cannot affect its parameters, i.e., Y is nondesignable. The function f maps the component space $(\mathcal{X}, \mathcal{Y})$ onto the specification space $\mathcal{Z}$, such that if $z = f(x, y) \in \mathcal{B}$, then the realization (x, y) is said to meet the specification. $\mathcal{B}$ is furthermore allowed to change according to some independent parameter, in which case the optimal θ will also depend on that parameter. The reason for this assumption will be apparent in Section VI.

Since (x, y) are samples of (X, Y), z will be samples of the random variable $f(X, Y)$, and by changing θ under $\mathcal{G}$, we will affect the sampling distribution in $\mathcal{Z}$. Thus by examining the outcomes z in $\mathcal{Z}$, we can, at least in principle, decide which θ are optimal, i.e., minimize $c(\theta, \mathcal{G})$.

In a general sense, the design process includes not only the determination of θ, but also $f(x, y)$, n, and $c(\theta, \mathcal{G})$, corresponding to the structure, order, and "best" criterion, respectively. In fact, even $\mathcal{B}$ is a designable parameter in many cases, since specifications cannot always be stated unambiguously. However, in this paper we shall consider f, n, c, and $\mathcal{B}$ given and concentrate on θ only.

A. Generalized Regions

The basic problem we will be concerned with is to somehow localize and describe the image of the specification space $\mathcal{B}$ in the component space $(\mathcal{X}, \mathcal{Y})$ as defined by

$$\mathcal{A}_0 = f^{-1}(\mathcal{B}) = \{(x, y): f(x, y) \in \mathcal{B}\} \subset (\mathcal{X}, \mathcal{Y}). \quad (2.1)$$

It is evident that this region plays a fundamental role when determining the optimal θ values. However, we cannot hope to gain complete knowledge about $\mathcal{A}_0$ other than in very simple cases, and usually this is not necessary.

To this end, we will first reformulate our problem slightly. Since we cannot affect the Y distribution, it is preferable to work in the $\mathcal{X}$ space only. To achieve this we introduce the function $\varphi(x)$ by

$$\varphi(x) = \Pr\{(X, Y) \in \mathcal{A}_0 / X = x\} \quad (2.2)$$

i.e., $\varphi(x)$ is the conditional probability that a sample (x, y)

of (X, Y) will have $z=f(x, y)\in\mathfrak{B}$, given $X=x$.

In many cases the influence of the Y variables is deterministic, in which case

$$\varphi(x)=\begin{cases}1, & x\in\mathcal{Q}_0\\ 0, & x\notin\mathcal{Q}_0.\end{cases} \tag{2.3}$$

However, in order to treat also the optimization of random functions $f(x, Y)$, we will allow $\varphi(x)$ to take values between 0 and 1.

To get a better picture of this situation, we form a new region $\mathcal{Q}$, which we will call a generalized region, in the following way:

Divide the $\mathcal{X}$-space in unit cells Δx, with a "mesh" that becomes progressively finer as the approximation is improved. Then define a subregion $\Delta\mathcal{Q}(x_i)$ of each unit cell such that

$$\int_{\Delta\mathcal{Q}(x_i)} dx=\varphi(x_i)\int_{\Delta x} dx \tag{2.4}$$

i.e., $\Delta\mathcal{Q}(x_i)$ is a region with a volume $\varphi(x_i)$ times that of Δx, but otherwise unspecified.

$\mathcal{Q}$ is now taken as the union of all $\Delta\mathcal{Q}(x_i)$:

$$\mathcal{Q}=\bigcup_i \Delta\mathcal{Q}(x_i). \tag{2.5}$$

Thus if $\varphi(x_i)=0$, no part of the unit cell at x_i belongs to $\mathcal{Q}$, while if $\varphi(x_i)=1$, the entire unit cell belongs to $\mathcal{Q}$. It is clear that every operation we can perform of $\mathcal{Q}_0$ is approximated by the same operation on $\mathcal{Q}$. In this way we can still speak of a well-defined region when random functions are involved.

The region $\mathcal{Q}$ will occasionally be a very scattered one, since each unit cell has one part that belongs to it, and another part that does not. It can be thought upon as having an "archipelagic" structure, where the amount of scattering is determined by $\varphi(x)$. It is evident that design problems comprising regions of this structure cannot easily be solved with methods assuming some kind of geometrical feature, such as for example convexity.

B. A Characterization of Generalized Regions

We are now faced with the problem of characterizing the region $\mathcal{Q}$ in such a way that we can draw conclusions about the optimal values of θ in different design situations. One such characterization could be

$$\mathcal{S}_a=\{V_a, \mu_a, M_a\}$$

$$V_a=\int_{\mathcal{Q}} dx$$

$$\mu_a=\int_{\mathcal{Q}} x\,dx/V_a$$

$$M_a=[m_a(i, j)],\qquad m_a(i, j)=\int_{\mathcal{Q}}(x_i-\mu_{ai})\cdot(x_j-\mu_{aj})\,dx/V_a. \tag{2.6}$$

This would give us information about the center (first-order moments μ_a) and extension (second-order moments M_a) of $\mathcal{Q}$. However, in order to carry out the integration, we must know $\mathcal{Q}$ and, as pointed out earlier, we do not have this knowledge in general. One way to evaluate the integrals would be by sampling from a uniform distribution that encloses $\mathcal{Q}$, but this requires at least some information about $\mathcal{Q}$. Since we do not want to assume such an information, we will choose the following more general characterization:

$$\mathcal{S}^*=\{V(x), P, \mu^*, M^*\}$$

where $V(x)$ is a measure over $\mathcal{Q}$ and

$$P=\int_{\mathcal{Q}} dV(x)$$

$$\mu^*=\int_{\mathcal{Q}} x\,dV(x)/P$$

$$M^*=[m^*(i, j)],\qquad m^*(i, j)=\int_{\mathcal{Q}}(x_i-\mu_i)\cdot(x_j-\mu_j)\,dV(x)/P. \tag{2.7}$$

Since the integrals are to be evaluated by sampling, we will choose $V(x)$ as a probability function, which means that

$$\int_{\mathcal{X}} dV(x)=1.$$

Of course there are many possible choices for $V(x)$, and this question will be settled next.

III. Optimal Measures

When deciding on an optimal measure $V(x)$, we must consider the following:

We have little or no *a priori* knowledge about $\mathcal{Q}$.
$\mathcal{Q}$ can be highly irregular.
$\mathcal{Q}$ may change according to an independent parameter since we allow $\mathfrak{B}$ to change.

In this situation, it is evident that one property of $V(x)$ must be a high dispersion, or ability to "look" in as many areas of the component space as possible.

In order to compare different choices of $V(x)$ with respect to dispersion, we must find a function $\mathcal{H}(X)$ that somehow quantifies this property. In doing so, we will take a similar approach as in [20]. We begin by dividing the component space in unit cells as before, and let $\mathcal{H}$ be the number of cells that a certain distribution covers. In order to make the comparison meaningful, we will also put the constraint of equal second-order moments on the different $V(x)$.

To this end we define the probability measure $\{p(x_i)\}$ from the frequency function $v(x)$ of X:

$$p(x_i)=p_i=v(x_i)\Delta x$$

$$v(x)=dV(x)/dx$$

$$\lim_{\Delta x\to 0}\sum_i v(x_i)\Delta x=1. \tag{3.1}$$

We can now state a number of postulates, that $\mathcal{H}$ should

fulfill in order to be a useful measure of dispersion. These are:

Postulate 1: $\mathcal{H}(X)$ is a function of $\{p_i\}$ only.
Postulate 2: $\mathcal{H}(X) \geq 1$ (since at least one cell has to be covered).
Postulate 3: If one or more cells with $p_i = 0$ is added, then $\mathcal{H}(X)$ will remain unchanged.
Postulate 4: $\mathcal{H}(X)$ is an increasing function of some integer n if $p_i = 1/n$ or 0 for all i.

We will need a fifth postulate that enables us to handle two distributions X and Y that may depend on each other. Thus if X and Y are independent, it is reasonable that the dispersion measure $\mathcal{H}(XY)$ of the combined distribution (XY) should be the product of the individual measures. In that case we will have

$$\mathcal{H}(XY) = \mathcal{H}(X)\mathcal{H}(Y). \tag{3.2}$$

On the other hand, if Y is completely determined by X, no extra cells will be covered by Y. This gives

$$\mathcal{H}(XY) = \mathcal{H}(X). \tag{3.3}$$

In situations between these extremes, we will use the function $\mathcal{H}(Y/X)$ as a measure of the dispersion in Y, given X. It is clear that $\mathcal{H}(XY)$ must depend on the conditional probabilities $p(Y=y_j/X=x_i)$, for which we can also determine the dispersion $\mathcal{H}(Y/x_i)$.

As a definition of $\mathcal{H}(Y/X)$ we will choose the geometrical average of $\mathcal{H}(Y/x_i)$ (it turns out that if the algebraic average is used, all postulates cannot be fulfilled):

$$\mathcal{H}(Y/X) = \prod_i \mathcal{H}(Y/x_i)^{p_i}. \tag{3.4}$$

If Y is independent of X, we will get $p(y_j/x_i) = p(y_j)$ and thus

$$\mathcal{H}(Y/X) = \prod_i \mathcal{H}(Y)^{p_i} = \mathcal{H}(Y). \tag{3.5}$$

When Y depends completely on $\mathcal{X}$, we have $p(y_j/x_i) = 1$ for some j and equal to 0 for all other j. Thus we may put $\mathcal{H}(Y/x_i) = 1$, since only one cell will be covered for each X-value, and we get

$$\mathcal{H}(Y/X) = \prod_i 1^{p_i} = 1.$$

The extreme cases will be satisfied if we formulate our fifth postulate in the following way:

Postulate 5: $\mathcal{H}(XY) = \mathcal{H}(X)\mathcal{H}(Y/X)$.

It is shown in the Appendix that the only function satisfying all postulates is

$$\mathcal{H}(X) = \prod_i p(x_i)^{-p(x_i)} = \exp\left[-\sum_i v(x_i)\Delta x \log(v(x_i)\Delta x) \right]. \tag{3.6}$$

We would now like to pass on to continuous distributions $V(x)$. To do this we form the function

$$\psi(X) = \Delta x \mathcal{H}(X)$$

which expresses the volume (unit cell volume times number of cells) that $V(x)$ covers. We then have

$$\begin{aligned}\psi(X) &= \Delta x \exp\left[-\sum_i v(x_i)\log v(x_i)\Delta x \right. \\ &\quad \left. -\log \Delta x \sum_i v(x_i)\Delta x \right] \\ &= \Delta x \exp\left[-\sum_i v(x_i)\log v(x_i)\Delta x - \log \Delta x \cdot 1 \right] \\ &= \exp H(x)\end{aligned}$$

where

$$H(X) = -\int_{\mathcal{X}} v(x)\log v(x)\,dx. \tag{3.7}$$

Thus we want to maximize $H(X)$ (which is called the entropy of $V(x)$ in some contexts) with respect to $V(x)$ under the constraints of equal second-order moments. This problem has already been solved in [8], where it is shown that the Gaussian distribution has the highest $H(X)$ of all distributions with equal moments. Thus we will choose $v(x)$ as

$$\begin{aligned} v(x) &= (2\pi)^{-n/2}(\det M)^{-1/2}\exp Q \\ Q &= -\tfrac{1}{2}(x-\mu)^T M^{-1}(x-\mu). \end{aligned} \tag{3.8}$$

In Fig. 1, three different distributions with the same variance are depicted. It is evident that the Gaussian distribution covers a wider interval than the others.

A. Further Optimization of V(x)

It has been shown in the previous section that the Gaussian distribution has the highest value of H when compared for equal second-order moments. This gives it a high ability to discover the structure of $\mathcal{A}$ and adapt to possible changes of $\mathcal{A}$.

We must now decide more specifically how to use this distribution in connection with $\mathcal{A}$. One way would be to fix the determinant of M and to maximize P in $\mathcal{S}^*$ as defined by (2.7). This is equivalent to maximizing the yield at constant tolerance cost in the case of design centering. Anderson [23] has treated a similar problem for symmetric, convex regions showing that if the first-order moments of $V(x)$ is placed in the center of that region, then the yield will be maximized. This result is however not applicable to the general type of regions we are interested in, and we will, therefore, take a different approach.

Since we want to use $V(x)$ also for the optimization of general functions, we will focus our attention on the dual problem (dual in the sense of exchanging target function and constraints) of maximizing the determinant while keeping P, or the yield, constant. In Section VI, it will be shown that general function optimization corresponds to a varying $\mathcal{A}$, and in this case we can expect the convergence to be better with the dual problem. This is of course due to the fact that maximizing the determinant of M is equivalent to expanding the distribution as much as possible over $\mathcal{A}$, and adjusting it to the shape of $\mathcal{A}$.

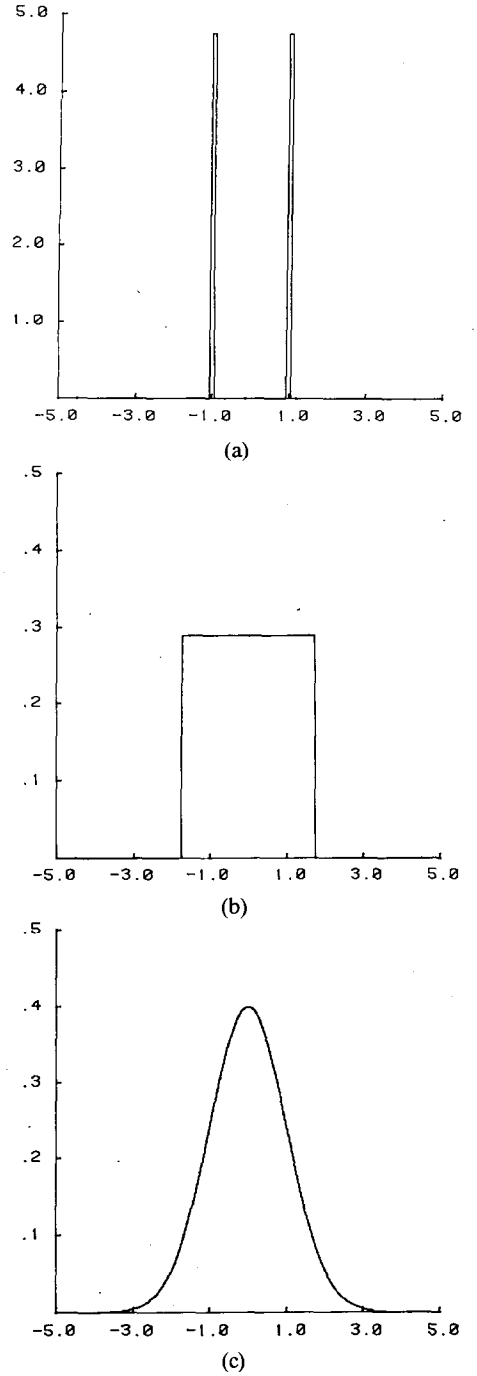

Fig. 1. Distributions with the same variance. (a) Dispersion=0.210. (b) Dispersion=3.46. (c) Dispersion=4.13.

For the Gaussian distribution, the expression for $H(X)$ is [8]

$$H=\log\{(2\pi e)^n \det(M)\}^{1/2}. \tag{3.9}$$

We can, therefore, choose to maximize either H or the determinant of M. More specifically, we will maximize the following Lagrange function w.r.t μ and $\{m(i,j)\}$:

$$F(\mu,\Lambda)=\log\left[(2\pi e)^n \det(M)\right]^{1/2}+\gamma(P-\alpha) + \sum_{i>j}\gamma_{ij}(\lambda_{ij}-\lambda_{ji}) \tag{3.10}$$

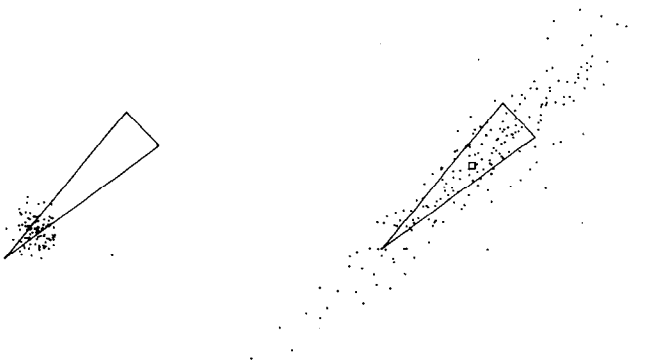

Fig. 2. Distributions with equal hitting probability (=0.3). The square marks center of gravity for the second distribution.

where

$$\Lambda=M^{-1}=[\lambda_{ij}], \qquad \gamma,\gamma_{ij}\text{: Lagrange multipliers.}$$

The maximizing conditions are derived in the Appendix, and they are as follows:

$$\mu=\mu^* \qquad M=cM^*, \quad c=\text{constant} \tag{3.11}$$

where μ^* and M^* are given by

$$\mu^*=[\mu_k^*], \qquad \mu_k^*=\int_{\mathcal{Q}} x_k v(x)\,dx/P$$

$$M^*=[m_{ij}^*], \qquad m_{ij}^*=\int_{\mathcal{Q}}(x_i-\mu_i)(x_j-\mu_j)v(x)\,dx/P. \tag{3.12}$$

It should be pointed out that while these results are theoretically valid only for Gaussian distributions, they may be used for other distributions as well, since these can often be approximated by Gaussian distributions. This is especially true if the number of dimensions is large (due to the central limit theorem).

The equations in (3.11) can be interpreted in the following way:

> The first-order moments μ of the distribution $V(x)$ should coincide with the center of gravity μ^* of the "success" sample points, i.e., those samples $x\in\mathcal{Q}$.
> The second-order moments $\{m(i,j)\}$ should be proportional to the second-order moments $\{m^*(i,j)\}$ of the same points.

In essence, this means that $V(x)$ will adapt to the location and shape of $\mathcal{Q}$ (see Fig. 2.). The question of how to achieve this in the most efficient way still remains.

IV. Implementation

The process is presently implemented in the following way:

1) $M=I_n$ — I_n is the unit matrix of order n.
   $Q=I_n$ — Q is given by $M=(rQ)(rQ)^T$ where r is an adaptable step size whose initial value is 1.

$\mu=\mu_0$	μ_0 is the starting values of the first-order moments.
2) $\eta\leftarrow\mathcal{N}(0, I_n)$	η is a sample from a Gaussian distribution with mean 0 and moment matrix I_n. θ should be read: "takes the value of."
3) $x\leftarrow\mu+r\cdot Q\cdot\eta$	A sample from the Gaussian distribution $V(x)\in\mathcal{N}(\mu, M)$ is taken.
$y\leftarrow Y$	y is sampled from the Y-distribution.
4) $f(x, y)$ is evaluated	
5) If $f(x, y)\notin\mathfrak{B}$ then	
$r\leftarrow r\cdot sf$	sf is a contraction factor (defined below).
Go to step 2	
6) If $f(x, y)\in\mathfrak{B}$ then	
$r\leftarrow r\cdot ss$	ss is an expansion factor (defined below).
$\mu\leftarrow(1-1/N_\mu)\mu+x/N_\mu$	μ is updated.
$\Delta M\leftarrow(1-1/N_M)I_n+\eta\cdot\eta^T/N_M$	ΔM can be regarded as an incremental change of the moment matrix.
$\Delta Q\leftarrow(\Delta M)^{1/2}$	ΔQ is defined by $\Delta M=\Delta Q\cdot\Delta Q^T$. Numerically, ΔQ can be found by the Cholesky method.
$Q\leftarrow Q\cdot\Delta Q$	Q is updated (and thus indirectly M).
$\det(Q)\leftarrow 1$	Q is normalized such that the determinant of Q equals 1.
Go to step 2.	

N_μ and N_M are weighting factors expressing the importance of previous samples. If these factors are approaching infinity, the moments will not be updated at all, and if they are 1, only the last sample will contribute.

The updating of M could have been done directly by

$$M\leftarrow(1-1/N_M)M+(\mu-x)(\mu-x)^T/N_M$$

but the procedure above (which is analytically equivalent) has turned out to be numerically more stable when the order n is high and the moment matrix is heavily skewed.

The expansion and contraction factors ss and sf are to be determined such that P is kept at a constant level. This means that the average value of $\det(M)$ should not change during stationary conditions (μ and M do not change). Since $\det(M)=r^{2n}\det(QQ^T)$ it is expanded with a factor ss^{2n} at each success sample and contracted with the factor sf^{2n} at each fail sample. After say S success samples and F fail samples the following relation must then be valid:

$$\prod_{i=1}^{S}(ss)^{2n}\prod_{i=1}^{F}(sf)^{2n}=1. \tag{4.1}$$

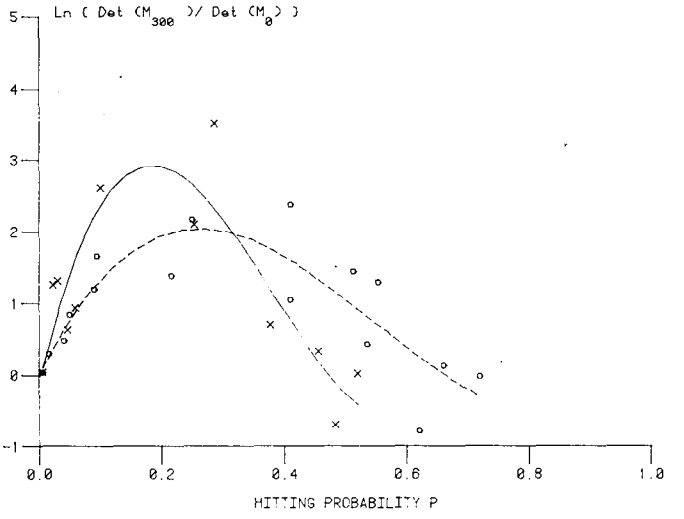

Fig. 3. Convergence of the process in a cylinder. Number of variables=6, number of samples=300. x: Weight $N_\mu, N_M=3$. —— : Least squares fitted 4th degree polynomial. o: Weight $N_\mu, N_M=6$. ---: Least squares fitted 4th degree polynomial.

Also

$$P=S/(S+F) \tag{4.2}$$

which after some calculation (assuming that ss and sf will be near 1) results in the approximate values

$$ss=1.+\beta*(1-P)$$
$$sf=1.-\beta*P.$$

The factor β determines the rate of contraction and expansion of the determinant. If it is too large, the process will exhibit a "pulsating" nature, which will disturb the convergence. On the other hand, if β is too small, the process becomes inert, and convergence will slow down.

V. Convergence of the Process

One feature of the process described is that its efficiency depends on a number of parameters (P, N_μ, N_M, β, etc.) that are difficult to determine theoretically. Because of this, different test environments must be constructed, in which the influence of these factors can be experimentally studied.

To begin with, it is clear that the value of P, or the "hitting" probability will greatly affect the convergence of the process. Thus if P approaches 1, the process will not be able to move at all, and if P goes to 0, no samples will hit $\mathfrak{A}$. One possible approach to determine the optimal value of P, is to consider the concept of useful information [15]. If we take the event scheme of hit versus no hit, and recall that the updating of the moments of the process is done only at hit, we will have the useful information

$$W=-P\log P \tag{5.1}$$

in which case the optimal P-value should be $1/e=0.37$. Other theoretical studies of the convergence in certain special cases also result in (5.1) [9].

Experimentally, this can be tested by for example performing test runs in order to find out how fast the process adapts to the shape of certain regions for different values of P. In Fig. 3, the convergence in a six-dimensional

cylinder is shown for $N_\mu, N_M = 3$ and $N_\mu, N_M = 6$. On the ordinate is depicted the growth of the determinant of M for a specified number of samples in each run. This is a measure of how well the process has aligned itself along the main axis of the cylinder. As can be seen, the optimal value of P is between 0.2 and 0.4.

The significance of the weighting factors N_μ and N_M is a tradeoff between statistical accuracy (large values) and movability of the process (small values). During the initial parts of the optimization, the process must be able to move quickly from the starting point (possibly along sharp curved valleys) to the vicinity of the optimum. Thus small weighting factors are preferred. To get significant estimates of μ and M, however, the weights must be increased. This can be done at regular intervals during the optimization as the optimum is approached. It should also be noted that in most practical design situations, the element values need not be known to a great accuracy, which means relative small weights.

These properties of the process can also be seen in Fig. 3. The runs with $N_\mu, N_M = 3$ converges faster than those with $N_\mu, N_M = 6$ for smaller values of P, but when P becomes large, the statistical uncertainty has a greater impact on these runs.

Some findings inferred from numerous experiments are:

The convergence can be maintained even for small weights ($N_M = 2 * n$ or less and N_μ even 1; n being the number of variables) provided that P is sufficiently small (less than 0.4).

The optimum value of P is somewhere in the neighborhood of 0.3.

The factor β in the step-size adjustment should be around 0.05 and decreased as the number of variables increases.

VI. Optimization of General Functions

In nonlinear optimization, one usually has a set of system response functions $\mathcal{R} = \{r_1(x, y), r_2(x, y), \cdots, r_l(x, y)\}$ and a corresponding set of desired responses $\mathcal{D} = \{d_1, d_2, \cdots, d_l\}$. From these sets, $f(x, y)$ can for example be defined in its simplest forms as

$$f(x, y) = \max_i \{r_i(x, y) - d_i\} \tag{6.1}$$

or

$$f(x, y) = \sum_i (r_i(x, y) - d_i)^2. \tag{6.2}$$

With a general purpose optimization algorithm such as [1] or [12], $f(x, y)$ is then minimized.

In our formulation, we will define the specification $\mathcal{B}$ as the interval

$$\mathcal{B} = \{f(x, y): f(x, y) < C_0\} \subset \mathcal{Z}, \qquad C_0\text{: scalar parameter.} \tag{6.3}$$

Consequently, the $\mathcal{Q}_0$ region is defined by

$$\mathcal{Q}_0 = \{(x, y): f(x, y) < C_0\} \subset (\mathcal{X}, \mathcal{Y}) \tag{6.4}$$

which means that $\mathcal{Q}_0$ will now depend on the parameter C_0.

Since we assume that X and Y are random variables, $f(X, Y)$ will also be a random variable, and we must therefore formulate the optimization problem in probabilistic terms. One obvious formulation is to minimize the average of $f(X, Y)$, but this would require a certain number of samples for each evaluation of the objective function. Also, since the estimation of the average in itself is a random variable, an ordinary minimization method would not work well in this case.

Therefore, we shall use a formulation suitable for the search process described earlier. We will choose θ as the first-order moments of the distribution function $V(x)$ for X, and

Minimize C_0 w.r.t θ

under the constraint $\mathcal{G}$:

$$\mathcal{G} = \{\Pr\{f(X(\theta), Y) < C_0\} = P = \text{constant}\}. \tag{6.5}$$

This means that by decreasing C_0, we are contracting the $\mathcal{Q}_0$ region to those parts of the component space where we have a high probability of finding low values of $f(X, Y)$. It should be noted that if f is a deterministic function, then the $\mathcal{Q}_0$ region will eventually degenerate to the point space containing the optimal x point.

A crucial question is the rate of contraction. If this is done too fast, the search process will be "left behind," and if it is done too slowly, the convergence will also be slow. From experiments again we have found the following type of updating of C_0 suitable:

$$C_0 \leftarrow (1 - 1/N_C) C_0 + f(x, y)/N_C. \tag{6.6}$$

This updating is done only for success samples. If the weight N_C is equal to 1, C_0 equals the function value of the latest success sample, and if N_C goes to infinity, there is no contraction at all. The optimal value of N_C has also to be found experimentally.

Example: Minimize

$$f_1(x) = 20 - \sum_{i=1}^{8} (x_i + 0.5)^2 + \exp\left\{25\left(\sum_{i=1}^{8} x_i^2 - 8\right)\right\}. \tag{6.7}$$

This function has the shape of a tilted bottom of a bottle with a small hill in the middle. The results are summarized in Fig. 4. For comparison, we have included the Fletcher algorithm using differentials [12], which is necessary if we assume that the gradients cannot be calculated analytically.

In a situation like this, the statistical optimization compares favorably with the gradient method, also when the function is continuous and differentiable. This is due to the fact that the statistical method can "climb over" the hill, while the gradient method goes around it, following the bottom of the valley.

If noise is added to the objective function we will get curve number 3 of Fig. 4. The function is

$$f_2(x, Y) = f_1(x) + Y \tag{6.8}$$

where Y has a Gaussian distribution with mean 0 and variance 0.01. The efficiency of the statistical method is but little affected, while the gradient method does not work in this case without special arrangements.

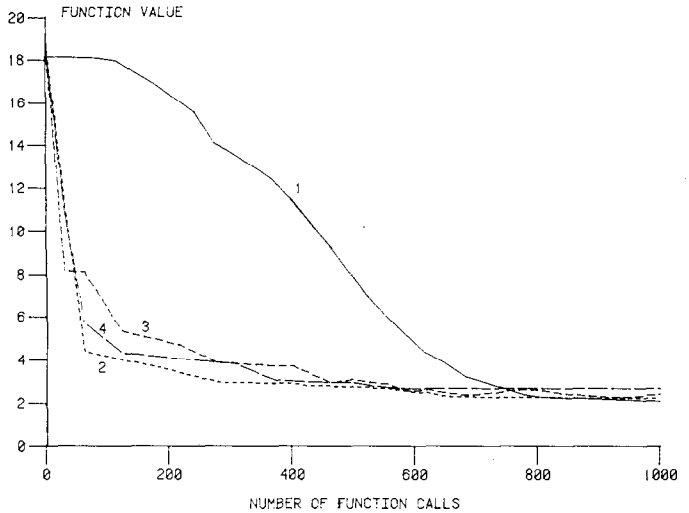

Fig. 4. Test function optimization. 1: Quasi-Newton (Fletcher). 2: Statistical optimization. 3: Statistical optimization with noise. 4: Statistical optimization with quantized variable values (step size $=2^{-3}$). Weights: $N_\mu=1$, $N_M=16$, $N_c=16$. All variables $=-1$. at start.

To see that the method works also on discontinuous functions, the variables are quantized with a step of 2^{-3} before the function evaluation. This will turn f_1 into a "stair-case" function. It can be seen that this optimization is as fast as the continuous one.

If the sampling is done from a quantized version of the distribution $V(x)$, we have a discrete optimization that converges as good as the discontinuous optimization in this case. However, the best discrete point is seldom found in this way. To this end, the discrete optimization can be further developed by a technique similar to the one described in [16], where the eigenvectors of the gradient-optimization Hessian is used to generate linear search directions for the optimal discrete point.

We might use the inverse of the moment matrix M in the same way. However, search directions can also be directly generated by taking samples from the optimal distribution $V(x)$. It is then not necessary to find the eigenvectors of the inverse moment matrix. Also, we may use any definition of the objective function in contrast to [16], where the $L2$ norm must be used.

As an example, we have taken example number 3 of Steiglitz [17], which is a digital low-pass filter with 12 variables. The same filter has also been treated by Brglez [18]. We have used a denser frequency grid than Brglez towards the band edge, since the filter ripples are very close there. Using Steiglitz solution as a comparison, a number of runs with different random number seed produced the following results for a quantization step of 2^{-7}:

Max number of analyses in each run $=3000$.

Nv = Number of generated search directions.

Na = Number of analyses to find the best point in each run.

Fv = The value of the objective function ($Fv<1$ means an acceptable solution).

L = The distance to the best point with the distance to the nearest discrete point as unit.

Nv	Na	Fv	L
96	2363	1.0050	6
34	906	1.0647	4
83	1798	1.1247	7
43	1265	1.1181	7
53	2082	1.0890	14
30	959	1.1749	6
33	1282	1.0836	12
29	887	1.1056	11
Nearest point		2.2986	1
Steglitz point		0.99713	4
Continuous solution		0.877.	

The fact that many good points are found far away from the nearest one indicates that the search distribution has been able to adapt to the typical narrow valley form found in Chebyshev optimization of high degree filters.

VII. Design Centering and Tolerancing

By design centering and tolerancing we understand the process of assigning optimal nominal values and tolerances to the elements of a system according to some objective function, which in the most general case is a function of both the tolerances and the yield of the system [13], [19], [22]. When doing this, one has to keep in mind that the system will be affected by certain operational factors like heat, humidity and aging after the time of manufacturing. The problems associated with tolerances was recognized a long time ago (see, for example, [24]), but the common design procedure by that time was cut and try.

In our approach to this problem, the operational factors are represented by the Y-variables, which will now become a stochastic process $Y(t)$ with $t\in[0,T]$, where T is the life span of the system. We can now define $\varphi(x,t)$ as

$$\varphi(x,t)=\Pr\{s\in[0,t]:(X,Y(s))\in\mathcal{C}_0/X=x\} \quad (7.1)$$

which expresses the conditional probability that $(X,Y(t))$ will meet the specifications up to the time t, given $X=x$. We will also assume that $\varphi(x,0)=0$ or 1, thereby indicating that there is no uncertainty whether a system meets the requirement or not at the time of manufacturing.

We will now let $V(x)$ represent the statistical distribution of the system elements at $t=0$, and as designable parameters θ we will take the first- and second-order moments of V. The system requirement is stated in the same form as in the previous section.

Now for the same reasons as before, it is not possible directly to optimize the object or cost function as it is usually called in this context. However, all cost functions have in common that they try to assign as large as possible tolerances to the system elements, while keeping all other conditions unchanged.

We shall, therefore, formulate the optimization problem in the following way:

Maximize $\det(M)$ w.r.t θ under the constraint $\mathcal{G}$:

$$\mathcal{G}=\Pr\{t\in[0,T]:f(X(\theta),Y(t))<C_0\}$$
$$=P=\text{constant}. \quad (7.2)$$

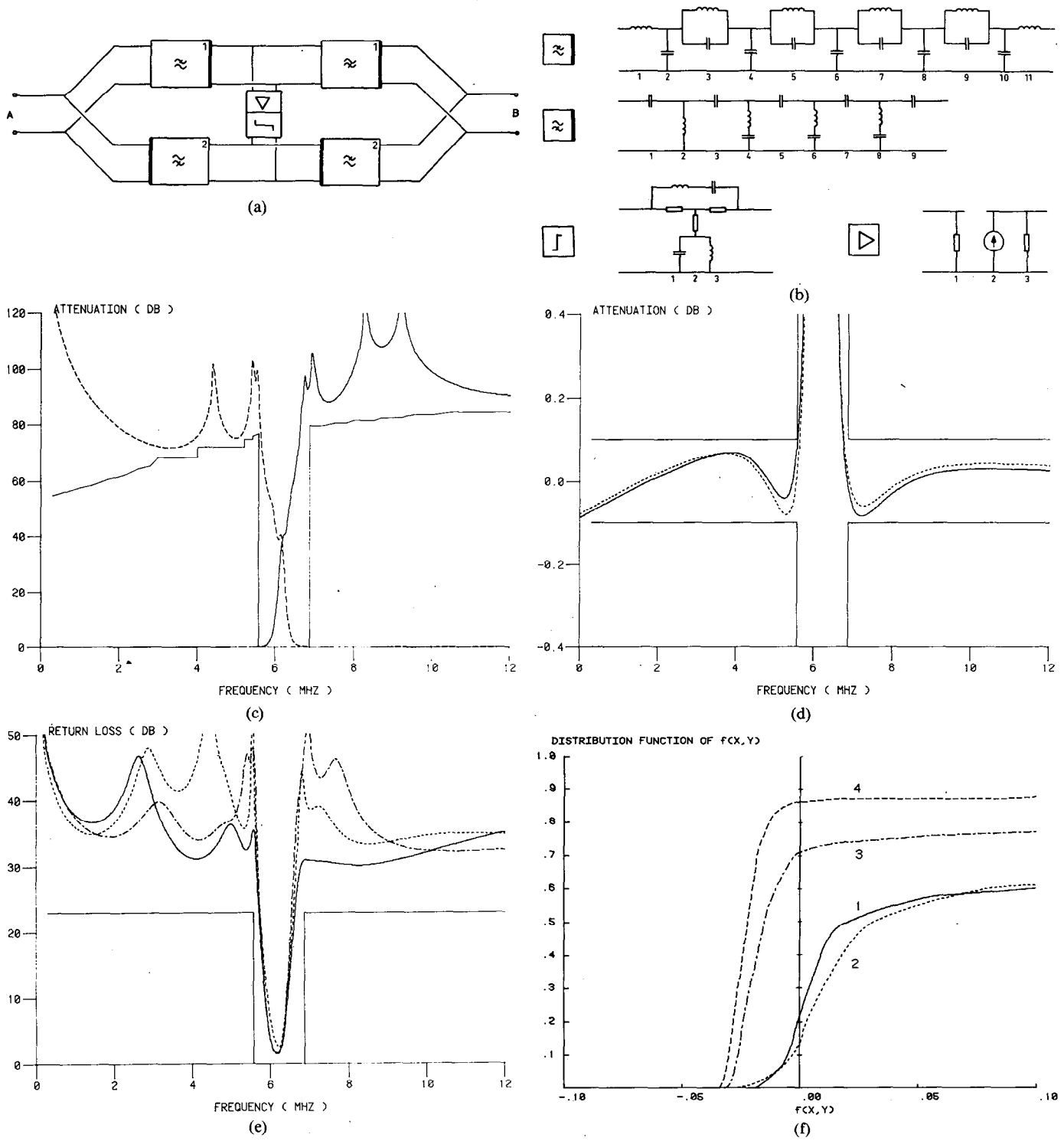

Fig. 5. (a) Directional filter arrangement. (b) Filter structures. (c) Stopband response. —— Low-pass direction --- High-pass direction. (d) Passband responses. —— Original response. --- Optimized response. (e) Return loss. —— Original response A and B side --- Optimized response A side - - - Optimized response B side. (f) Distribution of maximum error (sample size 300). 1: Manufacturing tolerances at start. 2: As 1 with environmental effects. 3: Design centering only. 4: Design centering and tolerancing.

This means as before that we will expand the $V(x)$ distribution as much as possible over the fixed $\mathcal{C}_0$ region, while keeping the probability of staying in that region constant.

Some remarks are relevant here. First, if the toleranced components are independent of each other, the M matrix is gradually made a diagonal matrix as the optimization proceeds. We can also use the residual standard deviations of $V(x)$ as a first approximation to the tolerances. Since the determinant of a diagonal matrix is the product of the diagonal elements, the tolerance cost function minimized is the sum of the logarithm of each individual tolerance. For other cost functions (like the sum of inverted tolerances) and different cost coefficients, other updating formulas similar to (3.11) can be derived [13].

TABLE I

	≈ 1 nom.	tol. %	≈ 2 nom.	tol. %
L1	2.9927	-	2.9927	-
C2	.4860	2.	.4860	2.
L3	1.8206	tuned F3	1.8206	tuned F3
C3	.2879	2.	.2879	2.
F3	6.9518	-	6.9518	-
C4	.4532	2.	.4532	2.
L5	3.0339	tuned F5	3.0399	tuned F5
C5	.09836	2.	.09836	2.
F5	9.2133	-	9.2133	-
C6	.4363	2.	.4363	2.
L7	1.7252	tuned F7	1.7252	tuned F7
C7	.3259	2.	.3259	2.
F7	6.7121	-	6.7121	-
C8	.3851	2.	.3851	2.
L9	2.4370	tuned F9	2.4370	tuned F9
C9	.1516	2.	.1516	2.
F9	8.2804	-	8.2804	-
C10	.5275	2.	.5275	2.
L11	2.9710	-	2.9710	-

	≈ 1 nom.	tol. %	≈ 2 nom.	tol. %
C1	.2149	2.	.2149	2.
L2	.9764	-	.9764	-
C3	.2282	2.	.2282	2.
C4	.4733	2.	.4733	2.
L4	1.8301	tuned F4	1.8301	tuned F4
F4	5.4076	-	5.4076	-
C5	.2735	2.	.2735	2.
C6	1.0149	2.	1.0149	2.
L6	1.2799	tuned F6	1.2799	tuned F6
F6	4.4159	-	4.4159	-
C7	.2936	2.	.2936	2.
C8	.3591	2.	.3591	2.
L8	2.3099	tuned F8	2.3099	tuned F8
F8	5.5260	-	5.5260	-
C9	.3550	2.	.3550	2.

∫ nom.	tol. %		▷ nom.	tol. %
L1 .9943	tuned F2	R1	75.	-
R1 6.5680	5.	B2	.03211	-
C1 .1767	2.	R3	75.	-
R2 424.96	5.			
C3 .6824	2.			
R3 6.5860	5.			
L3 3.8388	tuned F2			
F2 6.1100	-			

If the components are correlated, this can be considered either in the moment matrix or, in the case of complete correlation (tuning), as a functionally simple relationship between the components. Due to economical and practical reasons, it is usually not possible to use a sophisticated optimization algorithm to find the values of the tuned components.

Since the optimal value of P is close to 0.3 for maximum convergence, but in most cases in the neighborhood of 0.9 for minimum system cost, we must contract the achieved tolerances. This can be done by short Monte Carlo runs with the contraction as parameter to determine the minimum cost. In doing so, the Gaussian distribution may be replaced by some other desirable distribution.

Finally, the estimation of $\mathcal{G}$ would in principle require each realization of $Y(t)$ to be examined for every $t \in [0, T]$ to see whether the specification is violated or not. Since this is not possible, we have to limit ourselves to taking samples of these realizations by choosing some t in $[0, T]$. This could be done uniformly in the interval, or one could simply choose $t = T$, thereby assuming that the worst conditions exist at the end of the system life. The operational factors are sampled according to known statistics.

Example:

The system of Fig. 5(a) and 5(b) is a setup of directional filters with altogether 100 designable parameters (61 nominal values and 39 tolerances) and 22 nondesignable toleranced ones. Requirements and frequency responses are given in Fig. 5(c), 5(d), and 5(e). Fig. 5(f) shows the distribution of the objective function $f(X, Y)$ (according to 6.1) in different phases of the design process as estimated by Monte Carlo analysis. The requirements are met if $f(X, Y)$ is less than 0, and the yield is the value of the distribution function at that point.

It can be seen that the influence of the operational factors will decrease the yield from some 22 percent to below 14 percent at start. In the final design, this influence is very small.

After 4400 samples of the optimization (including the nondesignable operational factors), the yield has improved to about 86 percent, and the distribution curve is raised and moved to the left, which means that the solution is better suited to meeting different kinds of disturbances of the system elements. This is important, since the actual distributions involved are often not very well known. It can also be seen in Fig. 5(d) and 5(e) that the optimized responses have a greater margin towards the critical specification points.

The component values (in megahertz, microhenry, and nanofarads) and tolerances for the starting point are given

TABLE II

	≈ 1 nom.	tol. %	≈ 2 nom.	tol. %
L1	2.9970	-	2.9962	-
C2	.4719	2.065	.4839	1.979
L3	1.7070	tuned F3	1.7905	tuned F3
C3	.3014	1.729	.2931	2.189
F3	7.0166	-	6.9475	-
C4	.4330	2.364	.4547	1.989
L5	2.9207	tuned F5	2.9947	tuned F5
C5	.1001	1.604	.09950	1.790
F5	9.3080	-	9.2200	-
C6	.4281	1.666	.4389	2.067
L7	1.6569	tuned F7	1.7282	tuned F7
C7	.3415	2.793	.3248	2.222
F7	6.6980	-	6.7177	-
C8	.3851	1.825	.3824	2.081
L9	2.4387	tuned F9	2.4404	tuned F9
C9	.1535	2.023	.1515	2.222
F9	8.2260	-	8.2772	-
C10	.5338	2.511	.5279	2.005
L11	2.9350	-	2.9517	-

	≈ 1 nom.	tol. %	≈ 2 nom.	tol. %
C1	.2137	1.669	.2136	2.203
L2	.9794	-	.9767	-
C3	.2320	2.029	.2275	1.813
C4	.4781	2.137	.4771	2.444
L4	1.8078	tuned F4	1.8172	tuned F4
F4	5.4136	-	5.4053	-
C5	.2795	1.917	.2761	2.240
C6	.9615	1.878	1.0027	1.971
L6	1.3230	tuned F6	1.29319	tuned F6
F6	4.4623	-	4.4199	-
C7	.2835	2.152	.2953	1.918
C8	.3691	2.800	.3610	2.258
L8	2.2609	tuned F8	2.2941	tuned F8
F8	5.5094	-	5.5305	-
C9	.3372	2.436	.3529	1.738

	∫ nom.	tol. %	▷ nom.	tol. %
L1	1.0056	tuned F2	R1 75.	-
R1	6.5496	3.511	E2 .03206	-
C1	.1747	4.141	R3 75.	-
R2	422.94	1.945		
C3	.6804	2.028		
R3	6.4500	2.650		
L3	3.9165	tuned F2		
F2	6.0845	-		

in Table I, and in Table II the optimized nominal values and tolerances can be found. The Q-value of all inductors is 200 (tolerance $+-5$ percent), and the terminating impedances are both 75 Ω. All designs are compared for equal determinant or tolerance cost. More about this procedure can be found in [13] and [14].

Due to the complexity and size of this example, we have refrained from going into more details about it. For the interested reader, however, all information concerning element values for the different solutions, tuning procedures, environmental distributions, etc., can be obtained from the authors.

VIII. Conclusion

The development of a search process like the one described in this paper arises from the need for suitable design tools adapted to practical design problems in the telecommunication industry. The manufacturing and operational requirements are of major importance here due to economical reasons, and must be considered during the development of any method. Some consequences of this philosophy are:

The optimization should be capable of optimizing random functions.

Since the design problem often has a large number of designable parameters, the method must not be "dimension-sensitive," by which we mean that the optimization work should not increase exponentially with the number of parameters. On the other hand, the accuracy of the parameters need not often be more than 3 or 4 significant figures.

The method should be easily adapted to various design situations.

The design procedure presented here is an attempt to meet these requirements. We have demonstrated that it is possible to device a stochastic search process, that will work in various design situations. Needless to say, many questions still have to be answered, and other approaches can be taken. It is our hope, however, that future research will be carried out bearing in mind some of the questions raised here, and concentrate on methods that have a great potential in practical design situations.

Appendix

A. Structure of $\mathcal{H}$

Let m and r be natural numbers, and consider m independent sets of events $S_1, S_2, \cdots, S_m$ each containing r

equally probable events. We then have

$$\mathcal{H}(S_k)=\mathcal{H}(1/r,\cdots,1/r)=L(r). \quad \text{(A.1)}$$

This gives for the combined set of of events

$$\mathcal{H}(S_1S_2\cdots S_m)=\prod_k \mathcal{H}(S_k)=L^m(r) \quad \text{(A.2)}$$

according to postulate 5. On the other hand each event in the combined event has equal probability of occurrence $1/r^m$, which gives

$$L(r^m)=L^m(r). \quad \text{(A.3)}$$

Now choose s, r, n, and m such that

$$s^m<r^n<s^{m+1}.$$

Then

$$m\log(s)<n\log(r)<(m+1)\log(s)$$

$$m/n<\frac{\log(r)}{\log(s)}<(m+1)/n. \quad \text{(A.4)}$$

On the other hand, we have (from postulate 3)

$$L(s^m)<L(r^n)<L(s^{m+1})$$

$$L^m(s)<L^n(r)<L^{m+1}(s)$$

$$m\log L(s)<n\log L(r)<(m+1)\log L(s)$$

$$m/n<\frac{\log L(s)}{\log L(s)}<(m+1)/n. \quad \text{(A.5)}$$

Since these relationships must hold for all values of m and n, we get

$$\left|\frac{\log L(r)}{\log L(s)}-\frac{\log(r)}{\log(s)}\right|\leqslant 1/n. \quad \text{(A.6)}$$

This means that (as n approaches to infinity)

$$\frac{\log L(r)}{\log(r)}=\frac{\log L(s)}{\log(s)}=\lambda$$

or

$$L(r)=a^{\lambda^a\log(r)}. \quad \text{(A.7)}$$

We may without restrictions choose $\lambda=1$ and base e, which gives

$$L(n)=n. \quad \text{(A.8)}$$

Now let us define

$$p_k=g_k/g,\ \sum_k g_k=g, \qquad g_k, g \text{ natural numbers}$$

and introduce the set of events Y, consisting of n groups of events G_k, each containing g_k elements with equal probability of occurrence of $1/g_k$. We also assume that the event x_k implies that $y_j\in G_k$. We then have

$$p(y_j/x_k)=\begin{cases}0, & \text{if } y_j\notin G_k\\ 1/g_k, & \text{if } y_j\in G_k\end{cases}$$

and

$$\mathcal{H}(Y/X_k)=\mathcal{H}(1/g_k,\cdots,1/g_k)=L(g_k)=g_k=p_k\cdot g$$

$$\mathcal{H}(Y/X)=\prod_k \mathcal{H}(Y/X_k)^{p_k}=\prod_k (p_k\cdot g)^{p_k}=g\prod_k p_k^{p_k}. \quad \text{(A.9)}$$

On the other hand, we have that the probability of occurrence of the event XY is p_k times $1/g_k$, which equals $1/g$, and thus

$$\mathcal{H}(XY)=L(g)=g$$

and according to Postulate 5,

$$\mathcal{H}(X)=\mathcal{H}(XY)/\mathcal{H}(Y/X)=\prod_k p_k^{-p_k}=e^{-\sum_k p_k\log p_k}. \quad \text{(A.10)}$$

It now remains to be shown that Postulate 5 holds for arbitrary probabilities:

$$\begin{aligned}\mathcal{H}(Y/X)&=\prod_k \mathcal{H}(Y/X_k)^{p(x_k)}\\ &=\prod_k\left[\prod_j p(y_j/x_k)^{-p(y_j/x_k)}\right]^{p(x_k)}\\ &=\prod_k\prod_j\left[p(y_jx_k)/p(x_k)\right]^{-p(y_jx_k)}\\ &=\prod_k\prod_j p(y_jx_k)^{-p(y_jx_k)}\prod_k\prod_j p(x_k)^{p(y_jx_k)}\\ &=\mathcal{H}(XY)\prod_k p(x_k)\sum_j p(y_jx_k)\\ &=\mathcal{H}(XY)\prod_k p(x_k)^{p(x_k)}\\ &=\mathcal{H}(XY)/\mathcal{H}(X).\end{aligned}$$

It is easily seen that the other postulates also hold.

B. Optimal Conditions for V(x)

In order to find the maximizing conditions for (3.9), we introduce the Lagrange function

$$F(\mu,\Lambda)=\log\left[(2\pi e)^n\det(M)\right]^{1/2}+\gamma(P-\alpha)+\sum_{i>j}\gamma_{ij}(\lambda_{ij}-\lambda_{ji}) \quad \text{(A.11)}$$

where

$$\Lambda=M^{-1}=[\lambda_{ij}]$$

$\gamma, \gamma_{ij}=$ Lagrange multipliers

$$P=\int_{\mathcal{Q}} v(x)\,dx$$

$$v(x)=(\det\Lambda)^{1/2}(2\pi)^{-n/2}e^{Q}$$

$$Q=-1/2(x^T-\mu^T)\Lambda(x-\mu).$$

We will also use

$$\det(M)=(\det\Lambda)^{-1}$$

$$\det(\Lambda)=\sum_{k=1}^{n}\lambda_{ik}c_{ik}$$

where c_{ik} is the cofactor of the element λ_{ik}. Also,

$$m_{ij}=c_{ij}/\det\Lambda.$$

Differentiating P w.r.t λ_{ij} gives

$$\frac{\partial F}{\partial \lambda_{ij}} = -\frac{1}{2}(\det \Lambda)^{-1}\frac{\partial(\det \Lambda)}{\partial \lambda_{ij}} + \gamma\frac{\partial p}{\partial \lambda_{ij}} + \begin{cases} \gamma_{ij}, & i>j \\ 0, & i=j \\ -\gamma_{ij}, & i<j \end{cases}$$

$$\frac{\partial \det \Lambda}{\partial \lambda_{ij}} = c_{ij}$$

$$\frac{\partial p}{\partial \lambda_{ij}} = \int_{\mathcal{Q}} \frac{\partial v(x)}{\partial \lambda_{ij}}\,dx$$

$$\frac{\partial v(x)}{\partial \lambda_{ij}} = (2\pi)^{-n/2}\left[(\det \Lambda)^{1/2}e^{Q}\cdot\frac{\partial Q}{\partial \lambda_{ij}} + \frac{1}{2}(\det \Lambda)^{-1/2}\frac{\partial(\det \Lambda)}{\partial \lambda_{ij}}e^{Q}\right]$$

$$= (2\pi)^{-n/2}(\det \Lambda)^{1/2}e^{Q}\cdot\left[\frac{\partial Q}{\partial \lambda_{ij}} + \frac{1}{2}(\det \Lambda)^{-1}\frac{\partial(\det \Lambda)}{\partial \lambda_{ij}}\right]$$

$$\frac{\partial Q}{\partial \lambda_{ij}} = -\frac{1}{2}(x^T-\mu^T)\frac{\partial \Lambda}{\partial \lambda_{ij}}(x-\mu) = -\frac{1}{2}(x_i-\mu_i)(x_j-\mu_j).$$

Thus we have

$$\frac{\partial v(x)}{\partial \lambda_{ij}} = v(x)\left[-\frac{1}{2}(x_i-\mu_i)(x_j-\mu_j)+\frac{1}{2}m_{ji}\right]$$

$$\frac{\partial F}{\partial \lambda_{ij}} = -\frac{1}{2}m_{ji} + \gamma\int_{\mathcal{Q}}\frac{1}{2}v(x)\cdot\left[m_{ji}-(x_i-\mu_i)(x_j-\mu_j)\right]dx + \begin{cases} \gamma_{ij}, & i>j \\ 0, & i=j \\ -\gamma_{ij}, & i<j \end{cases}$$

$$= \frac{1}{2}m_{ji} + \frac{1}{2}\gamma P(m_{ji}-m_{ij}^*) + \begin{cases} \gamma_{ij}, & i>j \\ 0, & i=j \\ -\gamma_{ij} & i<j \end{cases} \tag{A.12}$$

$$m_{ij}^* = \frac{\int_{\mathcal{Q}}(x_i-\mu_i)(x_j-\mu_j)v(x)\,dx}{\int_{\mathcal{Q}}v(x)\,dx}. \tag{A.13}$$

Differentiating F w.r.t μ_i yields

$$\frac{\partial F}{\partial \mu_i} = \gamma\frac{\partial P}{\partial \mu_i}$$

$$\frac{\partial P}{\partial \mu_i} = \int_{\mathcal{Q}}\frac{\partial v(x)}{\partial \mu_i}\,dx$$

$$\frac{\partial v(x)}{\partial \mu_i} = (2\pi)^{-n/2}(\det \Lambda)^{1/2}e^{Q}\cdot\left[\frac{1}{2}e_i^T\Lambda(x-\mu)+\frac{1}{2}(x^T-\mu^T)\Lambda(-e_i)\right]$$

$$= \frac{1}{2}v(x)\left[\sum_k \lambda_{ik}(x_k-\mu_k)+\sum_k \lambda_{ki}(x_k-\mu_k)\right]$$

$$= \frac{1}{2}v(x)\sum_k (x_k-\mu_k)(\lambda_{ik}+\lambda_{ki})$$

and thus

$$\frac{\partial F}{\partial \mu_i} = \gamma\int_{\mathcal{Q}}\frac{1}{2}v(x)\sum_k (x_k-\mu_k)(\lambda_{ik}+\lambda_{ki})\,dx = \gamma\frac{P}{2}\sum_k(\lambda_{ik}+\lambda_{ki})(\mu_k^*-\mu_k) \tag{A.14}$$

$$\mu_k^* = \frac{\int_{\mathcal{Q}}x_k v(x)\,dx}{\int_{\mathcal{Q}}v(x)\,dx}. \tag{A.15}$$

To summarize, we have

$$\frac{\partial F}{\partial \lambda_{ij}} = -\frac{m_{ji}}{2} + \gamma\frac{P}{2}\left[m_{ji}-m_{ij}^*\right] + \begin{cases} \gamma_{ij}, & i>j \\ 0, & i=j=0 \\ -\gamma_{ij}, & i<j \end{cases}$$

$$\frac{\partial F}{\partial \mu_i} = \gamma\frac{P}{2}\sum_k(\lambda_{ik}+\lambda_{ki})(\mu_k^*-\mu_k) = 0$$

$$P=\alpha$$

$$\lambda_{ij}=\lambda_{ji} \quad \text{and} \quad m_{ij}=m_{ji}.$$

This will give us

$$-m_{ij}+\gamma P m_{ij}-\gamma P m_{ij}^* = 0$$

$$m_{ij} = \frac{\gamma P}{\gamma P-1}m_{ij}^*$$

$$\mu_i = \mu_i^*$$

$$P=\alpha$$

and, since P and γ are constants

$$M = cM^*$$

$$\mu = \mu^*. \tag{A.16}$$

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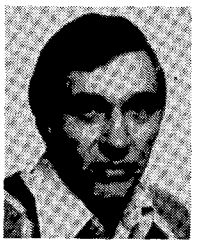

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