## Answers to Selected Exercises in Introduction to Stochastic Search and Optimization: Estimation, Simulation, and Control <br> by J. C. Spall

This section provides answers to selected exercises in the chapters and appendices. An asterisk (*) indicates that the solution here is incomplete relative to the information requested in the exercise. Unless indicated otherwise, the answers here are identical to those in the text on pp. 552-557 (it is possible that future versions of this site may include additional information, including solutions to supplementary exercises that are posted on the book's Web site).

## CHAPTERS 1-17

1.2. On the domain $[-1,1]$, the maximum occurs at $\theta=1 / \sqrt{5}$ and the minimum occurs at $\theta=-1$.
1.10.* The table below provides the solution for the first two (of six) iterations:

| $k$ | $\hat{\theta}_{k}^{T}$ | $L\left(\hat{\theta}_{k}\right)$ |
| :---: | :---: | :---: |
| 0 | $[0,3.0]$ | 52.0 |
| 1 | $[2.728,1.512]$ | 0.369 |
| 2 | $[2.500,1.228]$ | 0.0643 |

(Note: This problem corresponds to Example 8.6.2 in Bazaraa et al., 1993. The numbers here differ slightly from Bazaraa et al. This is apparently due to the limited accuracy used in Bazaraa et al.)
2.3.* A first-order Taylor approximation (Appendix A) yields

$$
\begin{aligned}
\log \left(1-P^{*}\right) & \approx \log (1)-\left.\frac{1}{1-P^{*}}\right|_{P^{*}=0} \times P^{*} \\
& =-P^{*} .
\end{aligned}
$$

This implies from (2.4) that the number of loss measurements $n$ satisfies $n=$ $\log \rho / \log \left(1-P^{*}\right) \approx-\log \rho / P^{*}$ for small $P^{*}$, as was to be shown.
3.4. (b) With $a=0.07$, the sample means of the terminal estimates for $\beta$ and $\gamma$ are 0.91 and 0.52 , respectively (versus true values of 0.90 and 0.50 ).
4.3.* The table below shows the sample means of the terminal estimate from 20 replications. Under each sample mean is the approximate 95 percent confidence interval using the principles in Section B. 1 (Appendix B).

|  | $n=100$ | $n=10,000$ | $n=1,000,000$ |
| :---: | :---: | :---: | :---: |
| Sample mean of <br> terminal <br> estimate (and <br> $95 \%$ interval) | 0.729 <br> $[0.700,0.760]$ | 0.920 <br> $[0.906,0.934]$ | 0.974 |
| $[0.970,0.977]$ |  |  |  |

5.10.* The table below presents the solution for the recursive processing with one pass through the data for one value of $a$. The mean absolute deviation (MAD) is computed with respect to the test data in reeddata-test.
6.4. For convenience, let $\boldsymbol{X}_{k}=k^{\beta / 2}\left(\hat{\boldsymbol{\theta}}_{k}-\theta^{*}\right)$. It is assumed that $\boldsymbol{X}_{k}$ converges in distribution to $N\left(\mu_{\mathrm{FD}}, \Sigma_{\mathrm{FD}}\right)$. From Figure C. 1 in Appendix C, pr. and a.s. convergence are both stronger than dist. convergence. However, even pr. and a.s. convergence, in general, are not strong enough to guarantee that the mean of the process converges (see Example C.4). Therefore, $E\left(\boldsymbol{X}_{k}\right) \rightarrow \mu_{\mathrm{FD}}$ in general.
7.3. With valid (Bernoulli) perturbations, the mean terminal loss value $L\left(\hat{\theta}_{1000}\right)$ is approximately 0.03 over several independent replications. For the (invalid) uniform $[-\sqrt{3}, \sqrt{3}]$ and $N(0,1)$ perturbation distributions, the $\theta$ estimate quickly diverges. Based on several runs, the terminal loss value was typically between $10^{50}$ and $10^{100}$ for the uniform case and much greater than $10^{100}$ for the normal case. This illustrates the danger of using an invalid perturbation distribution, even one that has the same mean and variance as a valid distribution.
8.6. SAN is run with the coefficients of Example 8.2 on the indicated two-dimensional quartic loss function. The table below shows the sample-mean terminal loss values for initial temperatures of $0.001,0.10$, and 10.0 based on an average over 40 replications. The results for the lowest and highest initial temperature are poorer than the results in Table 8.2; the results for the intermediate initial temperature ( 0.10 ) are pulled directly from Table 8.2.

| $N$ | $T_{\text {init }}=$ <br> 0.001 | $T_{\text {init }}=$ <br> 0.10 | $T_{\text {init }}=$ <br> 10.0 |
| :---: | :--- | :---: | :---: |
| 100 | 3.71 | 0.091 | 8.75 |
| 1000 | 2.12 | 0.067 | 6.11 |
| 10,000 | 0.429 | 0.0024 | 0.141 |

9.7.* The probability of a given (selected) binary-coded chromosome being changed from one generation to the next is bounded above by $P($ crossover $\cup$ mutation), where the event "mutation" refers to at least one bit being mutated. (The probability is bounded above because crossover does not guarantee that the chromosome will be changed. For example, one-point crossover applied as indicated to the following two distinct chromosomes does not change either chromosome: [ $\left.\begin{array}{lllll}0 & 1 & 0 \mid & 1 & 1\end{array}\right]$ ] and $\left[\begin{array}{lllll}1 & 1 & 0 \mid & 1 & 1\end{array}\right]$.) Note that
$P($ crossover $\cup$ mutation $)$

$$
\begin{aligned}
& =P(\text { crossover })+P(\text { mutation })-P(\text { crossover } \cap \text { mutation }) \\
& =P_{c}+\left(1-\left(1-P_{m}\right)^{B}\right)-P_{c}\left(1-\left(1-P_{m}\right)^{B}\right) .
\end{aligned}
$$

The probability of passing intact is therefore bounded below by $1-P($ crossover $\cup$ mutation $)$. (Note: The solution above represents a clarification of the solution on p. 554 of the first printing of the text to reflect that the probability $P$ (crossover $\cup$ mutation) is an upper bound-versus equality-to the probability of change in the chromosome.)

## 10.8.* Applying Stirling's approximation for "large" $N$ and $B$ yields

$$
N_{P} \approx \frac{1}{\sqrt{2 \pi}}\left(1+\frac{2^{B}-1}{N}\right)^{N}\left(1+\frac{N}{2^{B}-1}\right)^{2^{B}-1}\left(\frac{1}{2^{B}-1}+\frac{1}{N}\right)^{1 / 2} .
$$

11.3. (b) One aspect suggesting that the online form in (11.11) is superior is that it uses the most recent parameter estimate for all evaluations on the right-hand side of the parameter update recursion. The alternative form of TD in this exercise uses older parameter estimates for some of the evaluations on the right-hand side. Another potential shortcoming noted by Sutton (1988) is that the differences in the predictions will be due to changes in both $\theta$ and the inputs (the $\boldsymbol{x}_{\tau}$ ), making it hard to isolate only the effects of interest. In contrast to the recursion of this exercise, the temporal difference in predictions on the right-hand side of the recursion in (11.11) is due solely to changes in the input values (since the parameter is the same in all predictions).
12.4. Under the null hypothesis, $L\left(\theta_{m}\right)=L\left(\theta_{j}\right)$ for all $j \neq m$. Further, $E\left(\delta_{m j}\right)=0$ for all $j \neq m$ by the assumption of a common mean for the noise terms. Then

$$
\begin{aligned}
\operatorname{cov}\left(\delta_{m j}, \delta_{m i}\right) & =E\left[\left(\bar{L}_{m}-\bar{L}_{j}\right)\left(\bar{L}_{m}-\bar{L}_{i}\right)\right] \\
& =E\left(\bar{L}_{m}^{2}\right)-E\left(\bar{L}_{j} \bar{L}_{m}\right)-E\left(\bar{L}_{i} \bar{L}_{m}\right)+E\left(\bar{L}_{i} \bar{L}_{j}\right) \\
& =\operatorname{var}\left(\bar{L}_{m}\right)
\end{aligned}
$$

where the last line follows by the mutual uncorrelatedness over all $i, j$, and $m$ (so, e.g., $E\left(\bar{L}_{j} \bar{L}_{m}\right)$ $=E\left(\bar{L}_{j}\right) E\left(\bar{L}_{m}\right)=\left[E\left(\bar{L}_{m}\right)\right]^{2}$ for $\left.j \neq m\right)$.
13.7. Using MS EXCEL and the data in reeddata-fit, we follow the approach outlined in Example 13.5 in terms of splitting the data into four pairs of fitting/testing subsets. The four MSE values are $0.092,0.146,0.157$, and 0.181 and the four MAD values are $0.261,0.328,0.323$, and 0.328 . The modified Table 13.3 is given below; the values in italics are from Table 13.3 (so only the last column is new). The full linear model produces the lowest RMS and MAD values.

|  | Full linear model <br> $(13.9)$ | Reduced linear <br> model (13.10) | Five-input linear <br> model |
| :---: | :---: | :---: | :---: |
| RMS | 0.327 | 0.386 | 0.379 |
| MAD | 0.266 | 0.306 | 0.310 |

14.7. (b) We approximate the CRN -based and non-CRN-based covariance matrices using the sample covariance matrix from $2 \times 10^{6}$ gradient approximations generated via Monte Carlo simulation (this large number is needed to get a stable estimate of the matrix). The approximate covariance matrices are as follows:

$$
\begin{gathered}
\mathrm{CRN}: \operatorname{cov}\left[\hat{\boldsymbol{g}}_{k}\left(\hat{\theta}_{k}\right) \mid \hat{\theta}_{k}\right] \approx\left[\begin{array}{cc}
445.2 & 44.5 \\
44.5 & 465.3
\end{array}\right], \\
\text { Non-CRN: } \operatorname{cov}\left[\hat{g}_{k}\left(\hat{\theta}_{k}\right) \mid \hat{\theta}_{k}\right] \approx\left[\begin{array}{cc}
5936.0 & 93.5 \\
93.5 & 5956.4
\end{array}\right] .
\end{gathered}
$$

The above show that for $c_{k}=0.1$, the CRN covariance matrix is much smaller (in the matrix sense) than the non-CRN covariance matrix.
15.3. We have $\log p_{V}(v \mid \theta)=\log p_{V}(v \mid \lambda)=v \log \lambda+(1-v) \log (1-\lambda)$. Hence, $\partial \log p_{V}(v \mid \lambda) / \partial \lambda$ $=v / \lambda-(1-v) /(1-\lambda)$. This simplifies to $\lambda^{-1}(\lambda-v) /(\lambda-1)$, as shown in the first component of $\partial \log p_{V}(v \mid \theta) / \partial \theta$ in Example 15.4. The second component in $\partial \log p_{V}(v \mid \theta) / \partial \theta$ is zero since there is no dependence of $p_{V}(v \mid \theta)$ on $\beta$. The final form for $\boldsymbol{Y}_{k}\left(\hat{\theta}_{k}\right)$ then follows immediately using expression (15.12).
16.4.* Let $\boldsymbol{X}$ be the current state value and $\boldsymbol{W}$ be the candidate point. The candidate point $\boldsymbol{W}$ is accepted with probability $\rho(\boldsymbol{X}, \boldsymbol{W})$. This probability is random as it is depends on $\boldsymbol{X}$ and $\boldsymbol{W}$. For
convenience, let $\pi(\boldsymbol{x}, \boldsymbol{w})=p(\boldsymbol{w}) q(\boldsymbol{x}) /[p(\boldsymbol{x}) q(\boldsymbol{w})]$ (so $\rho(\boldsymbol{x}, \boldsymbol{w})=\min \{\pi(\boldsymbol{x}, \boldsymbol{w}), 1\}$ according to (16.3)). The mean acceptance probability is given by

$$
E[\rho(\boldsymbol{X}, \boldsymbol{W})]=\int_{\pi(\boldsymbol{x}, \boldsymbol{w}) \geq 1} p(\boldsymbol{x}) q(\boldsymbol{w}) d \boldsymbol{x} d \boldsymbol{w}+\int_{\pi(\boldsymbol{x}, \boldsymbol{w})<1} \pi(\boldsymbol{x}, \boldsymbol{w}) p(\boldsymbol{x}) q(\boldsymbol{w}) d \boldsymbol{x} d \boldsymbol{w}
$$

After several steps involving the re-expression of the integrals above (reader should show these steps), it is found that $E[\rho(\boldsymbol{X}, \boldsymbol{W})]=2 \int_{\pi(x, \boldsymbol{w}) \geq 1} p(\boldsymbol{x}) q(\boldsymbol{w}) d \boldsymbol{x} d \boldsymbol{w}$. The result to be proved then follows in several more steps (reader to show) by invoking the given inequality $p(\boldsymbol{x}) \leq C q(\boldsymbol{x})$. (Incidentally, the form of M-H where $q(\boldsymbol{w} \mid \boldsymbol{x})=q(\boldsymbol{w})$ is sometimes called the independent $M-H$ sampler.)
16.6. For the bivariate setting here, the general expression in (16.9) simplifies considerably. In particular, $\mu_{i}=\mu_{i i}=0, \Sigma_{i, i}=\rho$, and $\Sigma_{i, i, i}=1$. Hence, the bivariate sampling for the Gibbs sampling procedure is:

$$
X_{k+1,1} \sim N\left(\rho X_{k 2}, 1-\rho^{2}\right) \text { and } X_{k+1,2} \sim N\left(\rho X_{k+1,1}, 1-\rho^{2}\right)
$$

17.7. This problem is a direct application of the bound in property (iii) as shown in Subsection 17.2.2. The bound yields $1.098 \leq \operatorname{det} \boldsymbol{M}\left(\xi_{n}^{*}\right) \leq 1.5$.
17.17. (a) As in Example 17.12, consider the information number at each measurement (instead of $F_{n}$ ). This value is $x^{2} e^{-2 \theta x}$. Hence, the modified $D$-optimal criterion is $\rho x^{2} \exp \left(-2 \theta_{1} x\right)+(1-\rho) x^{2} \cdot \exp \left(-2 \theta_{2} x\right)$. The derivative with respect to $x$ yields

$$
\rho\left[2 x \exp \left(-2 \theta_{1} x\right)-2 \theta_{1} x^{2} \exp \left(-2 \theta_{1} x\right)\right]+(1-\rho)\left[2 x \exp \left(-2 \theta_{2} x\right)-2 \theta_{2} x^{2} \exp \left(-2 \theta_{2} x\right)\right] .
$$

Simplifying and setting to zero yields the following transcendental equation for $x$ :

$$
\rho \exp \left(-2 \theta_{1} x\right)\left(1-\theta_{1} x\right)+(1-\rho) \exp \left(-2 \theta_{2} x\right)\left(1-\theta_{2} x\right)=0 .
$$

This is a starting point for finding the support point for the design; we also need to ensure that the solution is a maximum (not a minimum or saddlepoint).

## APPENDICES A - E

A.3. (b) A plot of $f(\theta, x)$ is given below. The plot depicts the continuity of $f(\theta, x)$ on $\Theta \times \Lambda$, but also illustrates that there are some "sharp edges" where the derivative will not be continuous. Hence, not all conditions of Theorem A. 3 are satisfied.

B.5.* With the exception of the choice of matrix square root, we follow the steps of Exercise B.4. Using the chol function in MATLAB, the upper triangular Cholesky factorization of the initial covariance matrix is $\left[\begin{array}{cc}1.0 & 0.8 \\ 0 & 0.6\end{array}\right]$. In transforming the data, note that $\left(\Sigma^{1 / 2}\right)^{T} \Sigma^{1 / 2}=\Sigma\left(\right.$ but $\Sigma^{1 / 2}\left(\Sigma^{1 / 2}\right)^{T} \neq$ $\Sigma!$ ). We find that the $t$-statistics are -0.742 and -0.734 for the matched and unmatched pairs, respectively. This leads to corresponding $P$-values (for a one-sided test) of 0.238 ( 9 degrees of freedom) and 0.236 ( 18 degrees of freedom), respectively. These values are close to one another. Hence, the merit of using the matched-pairs test has been almost totally lost as a result of the relatively low correlation here.
C.4. (b) Note that $E\left(\left\|\boldsymbol{X}_{k}-\boldsymbol{X}\right\|^{r}\right)=E\left(\left\|\boldsymbol{X}_{k}-\boldsymbol{X}\right\|^{r}\left\|\boldsymbol{X}_{k}-\boldsymbol{X}\right\|^{0}\right)$. Because $0<r<q$, the Hölder inequality can be applied to the right-hand side of this expression:

$$
\begin{aligned}
E\left(\left\|\boldsymbol{X}_{k}-\boldsymbol{X}\right\|^{r}\right) & \leq\left\{E\left[\left(\left\|\boldsymbol{X}_{k}-\boldsymbol{X}\right\|^{r}\right)^{q / r}\right]\right\}^{r / q}\left\{E\left[\left(\left\|\boldsymbol{X}_{k}-\boldsymbol{X}\right\|^{0}\right)^{q /(q-r)}\right]\right\}^{(q-r) / q} \\
& =\left\{E\left(\left\|\boldsymbol{X}_{k}-\boldsymbol{X}\right\|^{q}\right)\right\}^{r / q} \times 1 .
\end{aligned}
$$

But $E\left(\left\|\boldsymbol{X}_{k}-\boldsymbol{X}\right\|^{q}\right) \rightarrow 0$ as $k \rightarrow \infty$ by assumption, implying $E\left(\left\|\boldsymbol{X}_{k}-\boldsymbol{X}\right\|^{r}\right) \rightarrow 0$ from the bound above. This completes the proof.
D.1. Given $J_{0}=a=c=3$ and modulus $=5$, we have $J_{1}=a J_{0}+c(\bmod m)=(3 \times 3+3)(\bmod 5)=$ 2. Continuing the iterative process, it is found that $J_{4}=J_{0}$. Therefore, this generator has period 4, which is smaller than the modulus.
E.1. From the matrix $\boldsymbol{P}^{4}$ in Example E.2, we hypothesize that $\overline{\boldsymbol{p}}=[0.305,0.256,0.439]^{T}$. As a first check on the validity of this solution, note that the elements sum to unity. Based on the given
$\boldsymbol{P}$, it is then straightforward to check the defining relationship $\overline{\boldsymbol{p}}^{T}=\overline{\boldsymbol{p}}^{T} \boldsymbol{P}$ given in (E.2). This indicates that to within three digits, the hypothesized $\overline{\boldsymbol{p}}$ is, in fact, the actual $\overline{\boldsymbol{p}}$.

