4. *(This problem is more involved, and may require some extra study.)* Compute and graph the exact solution set $\Sigma(Y\boldsymbol{A}, Y\boldsymbol{B})$.

   *(Hint: The paper [181], the description and references in [201], or the description in [175, Ch. 6 and §3.4] may be helpful.)*

## 1.3 DERIVATIVES AND SLOPES

A primary use of interval derivative information is in bounding ranges or variations in functions over regions. This was seen directly in §1.1.7, Definition 1.6, in which a second order interval extension was derived. Such information is also crucial in *interval Newton methods*, which in turn are central to fast and memory-efficient verified global optimization algorithms.

However, it is not always necessary to use interval extensions of the derivative. In fact, there are two techniques that actually lead to tighter bounds. To understand these techniques, it is useful to introduce the concept of a *Lipschitz matrix* and a *slope matrix* for a function $\phi : \mathbb{R}^n \to \mathbb{R}$. There is also a subsidiary technique due to Hansen, leading to slope matrices, that gives narrower bounds for multivariate problems.

### 1.3.1 Interval Derivatives and Slope Matrices

**Definition 1.10** ( [175, p. 174], etc.) *Let $F : \mathbb{R}^n \to \mathbb{R}^m$. The matrix $\boldsymbol{A}$ is said to be a* Lipschitz matrix *for $F$ over $\boldsymbol{X}$ provided, for every $X \in \boldsymbol{X}$ and $Y \in \boldsymbol{X}$, $F(X) - F(Y) = A(X - Y)$ for some $A \in \boldsymbol{A}$.*

Consider

**Example 1.1** *Let*

$$\phi(x_1, x_2) = x_1^3/3 + x_2^3/3 + x_1.$$

*Then a Lipschitz matrix for $\phi$ over the box $\boldsymbol{X} = ([-.5, .5], [-.5, .5])^T$ is any natural interval extension for the gradient: $\boldsymbol{A} = \big([-.5, .5]^2 + 1, [-.5, .5]^2\big) = \big([1, 1.25], [0, .25]\big)$, while the corresponding mean value extension for $\phi$, centered at $\check{X} = (0, 0)^T$, is*

$$\boldsymbol{\phi}_2(\boldsymbol{X}, \check{X}) = 0 + \big([1, 1.25], [0, .25]\big) \begin{pmatrix} [-.5, .5] \\ [-.5, .5] \end{pmatrix} = [-.75, .75].$$

In fact, if $F : \boldsymbol{X} \subset \mathbb{IR}^n \to \mathbb{R}^m$, then a component-by-component interval extension of the Jacobi matrix of $F$ constitutes a Lipschitz matrix for $F$ over $\boldsymbol{X}$.

**Definition 1.11** *If $F : \boldsymbol{X} \subset \mathbb{IR}^n \to \mathbb{R}^m$, then $\boldsymbol{F}'(\boldsymbol{X})$ will denote any interval matrix whose components are natural interval extensions over $\boldsymbol{X}$ of corresponding components of the Jacobi matrix of $F$. Any such matrix will be called an* interval Jacobi matrix.

An alternate, weaker property is the following.

**Definition 1.12** *Let $F : \mathbb{R}^n \to \mathbb{R}^m$. The matrix $\boldsymbol{A}$ is said to be an* interval slope matrix *(or, more generally, a slope set) for $F$ over $\boldsymbol{X}$ and centered on the interval vector $\check{\boldsymbol{X}}$ if, for every $X \in \boldsymbol{X}$ and $\check{X} \in \check{\boldsymbol{X}}$,*

$$F(X) - F(\check{X}) = A(X - \check{X}) \quad \textit{for some } A \in \boldsymbol{A}.$$

*Any smallest such set of matrices satisfying this condition will be denoted by $\mathbf{S}^\sharp(F, \boldsymbol{X}, \check{\boldsymbol{X}})$. An interval vector that contains $\mathbf{S}^\sharp(F, \boldsymbol{X}, \check{\boldsymbol{X}})$ (generally a good computed outer estimate) will be denoted by $\mathbf{S}(F, \boldsymbol{X}, \check{\boldsymbol{X}})$.*

Often, but not always, $\check{\boldsymbol{X}}$ is a point or a very small box.

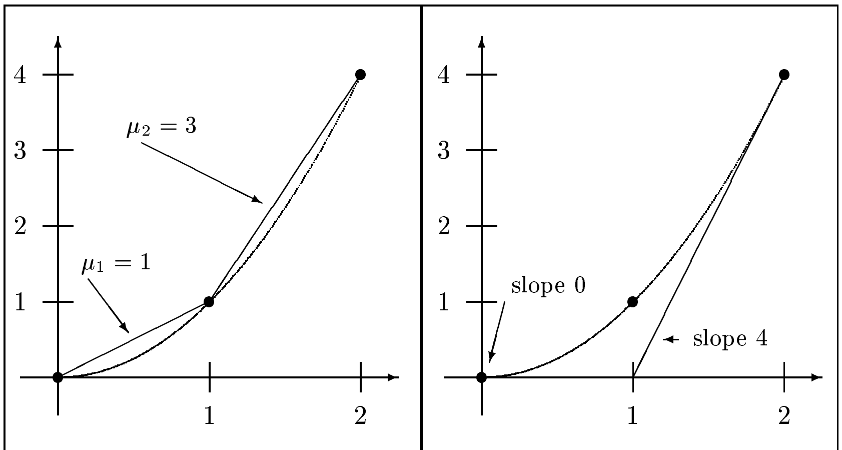
## *Univariate Slopes*

The difference between derivatives and slopes is most easily introduced with a one-dimensional example. For illustration purposes only, suppose a second-order extension to $f(x) = x^2$ is desired over the interval $[0, 2]$. Then the range of the derivative over $\boldsymbol{x} = [0, 2]$ is $\boldsymbol{a} = [0, 4]$, and the mean value extension, an enclosure for the range of $f(x) = x^2$ over $[0, 2]$, is:

$$f_2([0,2]) = f(1) + \boldsymbol{f}'([0,2])([0,2] - 1) = 1 + [0,4][-1,1] = [-3,5].$$

In contrast,

$$\boldsymbol{a} = \left\{ \mu \middle| \mu = \frac{x^2 - 1}{x - 1} \text{ for } x \in [0,2] \right\} = [1,3] = \mathbf{S}^\sharp(f, [0,2], 1)$$




(a) Range of slopes (b) Range of derivatives

**Figure 1.3** The difference between the interval slope $\mathbf{S}^\sharp(f, \boldsymbol{x}, \check{x})$ and the derivative range $\boldsymbol{f}'_u$ for $\boldsymbol{x} = [0, 2]$, $\check{x} = 1$ and $f(x) = x^2$

is a slope set for $f(x) = e^x$ over $\boldsymbol{x} = [-1, 1]$, centered[13] at $\check{x} = 0$. Because of that, $f_s(\boldsymbol{x}) = f(0) + [1, 2](\boldsymbol{x} - 1)$ is a second order extension of $f(x) = x^2$ for $\boldsymbol{x} \subseteq [0, 2]$, and an enclosure for the range of $f$ over $[0, 2]$ is

$$f_s([0, 2]) = 1 + [1, 3][-1, 1] = [-2, 4] \subset [-3, 5].$$

Figure 1.3 illustrates this relationship.

Although an interval extension would not actually be used for $f(x) = x^2$ (since the exact range is computable), this example illustrates a general relationship between derivatives and slopes, stated as

**Theorem 1.10** *Suppose $f : \mathbb{R} \to \mathbb{R}$, $\boldsymbol{x} \in \mathbb{IR}$ is arbitrary, and $\check{x} \in \boldsymbol{x}$. Suppose $\boldsymbol{f}'_u$ is the range of $f'$ over $\boldsymbol{x}$. Then*

$$\lim_{\mathrm{w}(\boldsymbol{x}) \to 0} \frac{\mathrm{w}\big(\boldsymbol{f}'_u(\boldsymbol{x})\big)}{\mathrm{w}\big(\mathbf{S}^\sharp(f, \boldsymbol{x}, \check{x})\big)} = 2.$$

Thus, slopes lead to narrower intervals than derivatives, where they are applicable.

[13]In fact, this particular $\boldsymbol{a}$ is the smallest such set satisfying Definition 1.12.

Theorem 1.10 is well known; its proof is not deep, and can be constructed from the following: $\mu \in \mathbf{S}(f, \boldsymbol{x}, \check{x})$ implies $\mu = (f(xf(\check{x}))/(x - \check{x}) = f''(c_2)(x - \check{x})$ for some $x \in \boldsymbol{x}$ and $c_2 \in \boldsymbol{x}$, while, for the same $x$, $f'(x) = f''(c_1)(x - \check{x})$ for some $c_1 \in \boldsymbol{x}$. Thus, $\mu/f'(x) = \frac{1}{2}\frac{f''(c_2)}{f''(c_1)} \approx \frac{1}{2}$, so $\mathbf{S}(f, \boldsymbol{x}, \check{x}) \approx 2\boldsymbol{f}'_u(\boldsymbol{x})$, and $\mathrm{w}(c[\underline{x}, \overline{x}]) = c\mathrm{w}([\underline{x}, \overline{x}])$.

In general, only enclosures for the range of the derivative and enclosures for the slope range $\mathbf{S}^\sharp(F, \boldsymbol{X}, \check{\boldsymbol{X}})$, not the exact ranges, can be computed, and the relationship between derivatives and slopes for multivariate functions is more complicated. However, with automatic differentiation as in §1.4 below, computation of derivative and slope enclosures are equally easy, and the computed slope enclosures are generally tighter than the derivative enclosures. Some comments and examples appear in [141], while a reference especially relevant for polynomials appears in [6]. In fact, Theorem 1.10 is a good rule of thumb for predicting the relative behavior of interval derivative and slope-based computations in a variety of settings.

## *Multivariate Slopes*

In Example 1.1 on page 26, a slope enclosure corresponding to a particular partial derivative of $\phi$ can be computed by simply treating the other variable as constant. For example, the second component of the slope matrix for $\phi$ over $\boldsymbol{X} = ([-.5, .5], [-.5, .5])^T$ can be computed as $\mathbf{S}(x^3/3, [-.5, .5], 0) \subset [0, .04167]$, rounded out to four digits. Similarly, with techniques of §1.4 below, the first component of the slope matrix can be computed as $[1, 1.04167]$, so $\boldsymbol{A} = \big([1, 1.25], [0, .25]\big)$ is a slope matrix for $\phi$ centered at $\check{X} = (0, 0)^T$ over $\boldsymbol{X}$, and a second-order interval extension of $\phi$ is

$$\begin{aligned} \boldsymbol{\phi}_s(\boldsymbol{X}) = 0 + \boldsymbol{A}(\boldsymbol{X} - \check{X}) &= \big([1, 1.08334], [0, .08334]\big) \begin{pmatrix} [-.5, .5] \\ [-.5, .5] \end{pmatrix} \\ &\subset [-.5834, .5834]. \end{aligned} \tag{1.23}$$

Here, $[-.5834, .5834] \subset [-.75, .75]$, where $[-.75, .75]$ is the enclosure obtained with the interval derivative, while the actual range of $\phi$, rounded out to four digits, is $\boldsymbol{\phi}^u(\boldsymbol{X}) \subset [-.5834, .5834]$, equal in this case to the enclosure given by slopes.

However, additional care must be taken when computing slopes of general multivariate functions. For example, if $\phi(X) = x_1^3 x_2^3$, with $\boldsymbol{X} = ([-.5, .5], [-.5, .5])^T$ and $\check{X} = (0, 0)^T$, one would be tempted to compute the first element of the slope enclosure by setting $x_2 \leftarrow \check{x}_2 = 0$, then using a univariate slope computation for $x_1$, and to similarly compute the second element by setting $x_1 \leftarrow \check{x}_1 = 0$. However, this would lead to the clearly incorrect[14] slope matrix of $\boldsymbol{A} = (0, 0)$. Thus, *in multivariate problems, variables other than the active one in computing a component of a slope matrix must be set to their interval, and not point, values.* This is crystallized in

**Algorithm 3** (Computation of a slope matrix)

INPUT: The function $\phi : \mathbb{R}^n \to \mathbb{R}$, the box $\boldsymbol{X}$ and the center $\check{\boldsymbol{X}}$, and a method of computing a slope bound $\mathbf{S}(f, \boldsymbol{x}, \check{\boldsymbol{x}})$ of a univariate function $f : \mathbb{R} \to \mathbb{R}$.

OUTPUT: A slope matrix $\boldsymbol{A} = \mathbf{S}(\phi, \boldsymbol{X}, \check{\boldsymbol{X}})$.

DO *for* $i = 1$ *to* $n$*:*

1. *Define* $f_i(x) = \boldsymbol{\phi}(\widehat{\boldsymbol{X}})$, *where* $\widehat{\boldsymbol{x}}_j = \boldsymbol{x}_j$ *for* $1 \le j \le n$, $j \ne i$ *and* $\widehat{\boldsymbol{x}}_i = x$, *where* $\boldsymbol{\phi}$ *is an interval extension of* $\phi$. *(Note that* $f_i$ *is in general an interval, even if* $x$ *is a point.)*
2. *Set* $\boldsymbol{a}_i$ *to the slope of the univariate function* $f_i$*:* $\boldsymbol{a}_i \leftarrow \mathbf{S}(f_i, \boldsymbol{x}_i, \check{\boldsymbol{x}}_i)$.

END DO

**End Algorithm 3**

### 1.3.2 Hansen's Slope Technique

In [73], and later in [77, §6.3–§6.4], Hansen explains a technique that allows use of point values for some of the variables, when computing derivative matrices for mean value type interval extensions. Hansen's slope technique is based on decomposing the change in $\phi : \mathbb{R}^n \to \mathbb{R}$ into changes in due to displacements along the coordinate directions, and on simple application of the mean value theorem. Different interval extensions are obtained depending on which displacements are considered first. For example, suppose $\phi : \mathbb{R}^2 \to \mathbb{R}$, and $\check{X} \in \boldsymbol{X} \subset \mathbb{IR}^2$. If displacement along the $x_1$ direction is considered first, cf. Fig. 1.4(a), then, for $(x_1, x_2) \in \boldsymbol{X}$,

$$\phi(x_1, x_2) = \phi(\check{x}_1, \check{x}_2) + \frac{\partial \phi}{\partial x_1}(c_1, \check{x}_2)(x_1 - \check{x}_1) + \frac{\partial \phi}{\partial x_2}(x_1, c_2)(x_2 - \check{x}_2), \quad (1.24)$$

[14] Use of this faulty slope matrix in an interval extension would lead to the conclusion that $\phi$ is constant on $\boldsymbol{X}$.