Analysis review: O notation, Taylor series, and linear algebra

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Introduction

One final lecture of analysis review, in which we go over three indispensable tools that we will use constantly in the remainder of the course:

- O, o notation
- Taylor series expansions
- Linear algebra

o-notation: Motivation

- When investigating the asymptotic behavior of functions, it is often convenient to replace unwieldy expressions with compact notation
- For example, if we encountered the mathematical expression

$$x^2 + a - a,$$

we would obviously want to replace it with x^2 since a - a = 0

• However, what if we encounter something like

$$x^2 + \frac{5\theta}{\sqrt{n}} - \frac{3\theta}{n+5}?$$

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• We can no longer just replace this with x^2

o-notation: Motivation (cont'd)

- However, as n gets larger, the expression gets closer and closer to x^2
- It would be convenient to have a shorthand notation for this, something like x^2+o_n , where o_n represents some quantity that becomes negligible as n becomes large
- This is the basic idea behind o-notation, and its simplifying powers become more apparent as the mathematical expression we are dealing with becomes more complicated:

$$\frac{x^2 + \frac{5\theta}{\sqrt{n}} - \frac{3\theta}{n+5}}{(n^2 + 5n - 2)/(n^2 - 3n + 1)} + \frac{\exp\{-\frac{1}{2} \|\mathbf{x} - \boldsymbol{\mu}\|^2\}}{2\sqrt{n}\theta \int_0^\infty g(s)ds}$$

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o-notation

- There is where something called o-notation comes in: a formal way of handling terms that effectively "cancel out" as we take limits
- **Definition:** A sequence of numbers X_n is said to be o(1) if it converges to zero. Likewise, X_n is said to be $o(r_n)$ if

$$\frac{X_n}{r_n} \to 0$$

as $n \to \infty$.

• When the rate is constant, o notation is pretty straightforward:

$$x^{2} + \frac{5\theta}{\sqrt{n}} - \frac{3\theta}{n+5} = x^{2} + o(1)$$

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o-notation remarks

- When the rate is not constant, expressions are a bit harder to think about – it helps to go over some cases:
- For example:
 - $\circ \ X_n \to \infty$, but $r_n \to \infty$ even faster:

$$n = o(n^2)$$

 $r_n \to 0$, but $X_n \to 0$ even faster:

$$\frac{1}{n^2} = o(1/n)$$

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 Note that this extension to non-constant rates are what makes o different from and more flexible than simpler statements about limits (convergence to a constant)

O-notation

- A very useful companion of o-notation is O-notation, which denotes whether or not a term remains bounded as $n \to \infty$
- **Definition:** A sequence of numbers X_n is said to be O(1) if there exist M and N such that

$$|X_n| < M$$

for all n > N. Likewise, X_n is said to be $O(r_n)$ if there exist M and N such that for all n > N,

$$\left| \frac{X_n}{r_n} \right| < M.$$

O-notation remarks

For example,

$$\frac{\exp\{-\frac{1}{2}\|\mathbf{x} - \boldsymbol{\mu}\|^2\}}{2\sqrt{n}\theta \int_0^\infty g(s)ds} = O(n^{-1/2})$$

- Note that $X_n = O(1)$ does not necessarily mean that X_n is bounded, just that it is eventually bounded
- Note also that just because a term is O(1), this does not necessarily mean that it has a limit; for example,

$$\sin\left(\frac{n\pi}{2}\right) = O(1),$$

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even though the sequence does not converge

O-notation remarks (cont'd)

- You may encounter the phrase " x_n is of order r_n "; this is a bit ambiguous
- The author may mean that $x_n = O(r_n)$
- However, it might also mean something stronger: that there exist constants m and M such that

$$m \le \left| \frac{x_n}{r_n} \right| \le M$$

for large enough n; i.e., the ratio is bounded above but also bounded below

• In other words, $x_n = O(r_n)$ but in addition $x_n \neq o(r_n)$; some authors use the notation $x_n \approx r_n$ to denote this situation

Informative-ness of o and O notation

- There are typically many ways of writing an expression using O
 notation, although not all of them will be equally informative
- For example, if $x_n = 1 + \frac{1}{n}$, then all of the following are true:

Algebra of O, o notation

 $O,o\mbox{-}{\rm notation}$ are useful in combination because simple rules govern how they interact with each other

Theorem: For $a \leq b$:

$$O(1) + O(1) = O(1)$$

$$o(1) + o(1) = o(1)$$

$$o(1) + O(1) = O(1)$$

$$O(1)O(1) = O(1)$$

$$O(1)O(1) = o(1)$$

$$O(1)O(1) = o(1)$$

$$O(n^{a}) + O(n^{b}) = O(n^{b})$$

$$O(n^{a}) + o(n^{b}) = o(n^{b})$$

Remarks

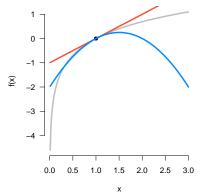
- O,o "equations" are meant to be read left-to-right; for example, $O(\sqrt{n})=O(n)$ is a valid statement, but $O(n)=O(\sqrt{n})$ is not
- Exercise: Determine the order of

$$n^{-2}\left\{(-1)^n\sqrt[n]{2}+(1+\frac{1}{n})^n\right\}.$$

- As we will see in a week or two, there are stochastic equivalents of these concepts, involving convergence in probability and being bounded in probability
- As such, we won't do a great deal with O, o-notation right now, but will use the stochastic equivalents extensively

Taylor series: Introduction

 As we will see (many times!), it is useful to be able to approximate a complicated function with a simple polynomial:



• This is the idea behind Taylor series expansions

Taylor series: Introduction (cont'd)

- It is difficult to overstate the importance of Taylor series expansions to statistical theory, and for that reason we are now going to cover them fairly extensively
- In particular, Taylor's theorem comes in a number of versions, and it is worth knowing several of them, since they come up in statistics quite often
- Furthermore, students often have not seen the multivariate versions of these expansions

Taylor's theorem

• Theorem (Taylor): Suppose n is a positive integer and $f: \mathbb{R} \to \mathbb{R}$ is n times differentiable at a point x_0 . Then

$$f(x) = \sum_{k=0}^{n} \frac{f^{(k)}(x_0)}{k!} (x - x_0)^k + R_n(x, x_0),$$

where the remainder R_n satisfies

$$R_n(x, x_0) = o(|x - x_0|^n) \text{ as } x \to x_0$$

- If $f^{(n+1)}(x_0)$ exists, you could also say that R_n is $O(|x-x_0|^{n+1})$
- This form of the remainder is sometimes called the Peano form

Taylor's theorem: Lagrange form

• Theorem (Taylor): Suppose $f: \mathbb{R} \to \mathbb{R}$ is n+1 times differentiable on an open interval containing x_0 . Then for any point x in that interval, there exists $\bar{x} \in (x, x_0)$:

$$R_n(x,x_0) = \frac{f^{(n+1)}(\bar{x})}{(n+1)!}(x-x_0)^{n+1}.$$

• This is also known as the *mean-value form*, as the mean value theorem is the central idea in proving the result

Comparing the two forms

 Comparing the Basic and Lagrange forms for a second-order expansion,

$$f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2}f''(x_0)(x - x_0)^2 + o(|x - x_0|^2)$$

$$f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2}f''(\bar{x})(x - x_0)^2$$

• We can see that in the second case, we have a simpler expression, but to obtain it, we require f'' to exist along the entire interval from x to x_0 , not just at the point x_0

Example: Absolute value

- For example, consider approximating the function f(x) = |x| at $x_0 = -0.1$
- Note that f' exists at x_0 , but not at 0
- The basic form of Taylor's theorem says that if we get close enough to x_0 , the approximation f(-0.1) + f'(-0.1)(x+0.1) becomes very accurate indeed, the remainder is exactly zero for any x within 0.1 of x_0
- However, suppose x=0.2; since f is not differentiable at zero, we are not guaranteed the existence of a point \bar{x} such that

$$f(0.2) = f(-0.1) + 0.3f'(\bar{x});$$

and indeed in this case no such point exists

Lagrange bound

- One reason why the Lagrange form is more powerful is that it allows us to establish error bounds to know exactly how close x must be to x_0 in order to ensure that the approximation error is less than ϵ
- In particular, if there exists an M such that $\left|f^{(n+1)}(x)\right| \leq M$ over the interval (x,x_0) , then

$$|R_n(x)| \le \frac{M}{(n+1)!} |x - x_0|^{n+1}$$

Multivariable forms of Taylor's theorem

- We now turn our attention to the multivariate case
- For the sake of clarity, I'll present the first- and second-order expansions for each of the previous forms, rather than abstract formulae involving $f^{(n)}$
- Lastly, I'll provide a form that goes out to third order, although higher orders are less convenient as they can't be represented compactly using vectors and matrices
- Note that these forms are only covering the case of scalar-valued functions $f: \mathbb{R}^d \to \mathbb{R}$; we will need results for the vector-valued case $f: \mathbb{R}^d \to \mathbb{R}^k$ as well, but we will go over that in a later lecture

Taylor's theorem

• Theorem (Taylor): Suppose $f: \mathbb{R}^d \to \mathbb{R}$ is differentiable at a point \mathbf{x}_0 . Then

$$f(\mathbf{x}) = f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)^{\mathsf{T}} (\mathbf{x} - \mathbf{x}_0) + o(\|\mathbf{x} - \mathbf{x}_0\|)$$

• Theorem (Taylor): Suppose $f: \mathbb{R}^d \to \mathbb{R}$ is twice differentiable at a point \mathbf{x}_0 . Then

$$f(\mathbf{x}) = f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)^{\top} (\mathbf{x} - \mathbf{x}_0) + \frac{1}{2} (\mathbf{x} - \mathbf{x}_0)^{\top} \nabla^2 f(\mathbf{x}_0) (\mathbf{x} - \mathbf{x}_0) + o(\|\mathbf{x} - \mathbf{x}_0\|^2)$$

Taylor's theorem: Lagrange form

• Theorem (Taylor): Suppose $f: \mathbb{R}^d \to \mathbb{R}$ is differentiable on $N_r(\mathbf{x}_0)$. Then for any $\mathbf{x} \in N_r(\mathbf{x}_0)$, there exists $\bar{\mathbf{x}}$ on the line segment connecting \mathbf{x} and \mathbf{x}_0 such that

$$f(\mathbf{x}) = f(\mathbf{x}_0) + \nabla f(\bar{\mathbf{x}})^{\top} (\mathbf{x} - \mathbf{x}_0)$$

• Theorem (Taylor): Suppose $f: \mathbb{R}^d \to \mathbb{R}$ is twice differentiable on $N_r(\mathbf{x}_0)$. Then for any $\mathbf{x} \in N_r(\mathbf{x}_0)$, there exists $\bar{\mathbf{x}}$ on the line segment connecting \mathbf{x} and \mathbf{x}_0 such that

$$f(\mathbf{x}) = f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)^{\top} (\mathbf{x} - \mathbf{x}_0) + \frac{1}{2} (\mathbf{x} - \mathbf{x}_0)^{\top} \nabla^2 f(\bar{\mathbf{x}}) (\mathbf{x} - \mathbf{x}_0)$$

• " $\bar{\mathbf{x}}$ on the line segment connecting \mathbf{x} and \mathbf{x}_0 " means that there exists $w \in [0,1]$ such that $\bar{\mathbf{x}} = w\mathbf{x} + (1-w)(\mathbf{x}_0)$

Taylor's theorem: Third order

Theorem (Taylor): Suppose $f: \mathbb{R}^d \to \mathbb{R}$ is three times differentiable on $N_r(\mathbf{x}_0)$. Then for any $\mathbf{x} \in N_r(\mathbf{x}_0)$, there exists $\bar{\mathbf{x}}$ on the line segment connecting \mathbf{x} and \mathbf{x}_0 such that

$$f(\mathbf{x}) = f(\mathbf{x}_0) + \sum_{j=1}^d \frac{\partial f(\mathbf{x}_0)}{\partial x_j} (x_j - x_{0j})$$

$$+ \frac{1}{2} \sum_{j=1}^d \sum_{k=1}^d \frac{\partial^2 f(\mathbf{x}_0)}{\partial x_j \partial x_k} (x_j - x_{0j}) (x_k - x_{0k})$$

$$+ \frac{1}{6} \sum_{j=1}^d \sum_{k=1}^d \sum_{\ell=1}^d \frac{\partial^3 f(\bar{\mathbf{x}})}{\partial x_j \partial x_k \partial x_\ell} (x_j - x_{0j}) (x_k - x_{0k}) (x_\ell - x_{0\ell}),$$

where $\partial f(\mathbf{x}_0)/\partial x_j$ is shorthand for $\partial f(\mathbf{x})/\partial x_j$ evaluated at \mathbf{x}_0

Linear algebra

- Our last mathematical topic to review/reference is linear algebra, which we will use right away in our next lecture on the multivariate normal distribution
- If this material is new to you, then I would encourage you to read this as well
- It is often useful to switch the rows and columns of a matrix around. The resulting matrix is called the *transpose* of the original matrix, and denoted with a superscript ^T or an apostrophe ':

$$\mathbf{M} = \begin{bmatrix} 3 & 2 \\ 4 & -1 \\ -1 & 2 \end{bmatrix} \qquad \mathbf{M}^{\mathsf{T}} = \begin{bmatrix} 3 & 4 & -1 \\ 2 & -1 & 2 \end{bmatrix}$$

Linear and quadratic forms

- Matrix products involving linear and quadratic forms come up very often in statistics, and it is important to have an intuitive grasp on what they represent
- Here are some useful identities/relationships involving matrix products and their scalar representations:

$$\mathbf{a}^{\top}\mathbf{x} = \sum_{i} a_{i}x_{i}; \quad \mathbf{1}^{\top}\mathbf{x} = \sum_{i} x_{i}$$

$$\mathbf{A}^{\top}\mathbf{x} = (\sum_{i} a_{i1}x_{i} \quad \cdots \quad \sum_{i} a_{ik}x_{i})^{\top}$$

$$\mathbf{a}^{\top}\mathbf{W}\mathbf{x} = \sum_{i} \sum_{j} a_{i}w_{ij}x_{j}; \quad \mathbf{a}^{\top}\mathbf{1}\mathbf{x} = \sum_{i} \sum_{j} a_{i}x_{j}$$

$$(\mathbf{AWB})_{ij} = \sum_{k} \sum_{m} a_{ik}w_{km}b_{mj}$$

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Inverses

- **Definition:** The *inverse* of an $n \times n$ matrix A, denoted A^{-1} , is the matrix satisfying $AA^{-1} = A^{-1}A = I_n$, where I_n is the $n \times n$ identity matrix.
- Note: We're sort of getting ahead of ourselves by saying that \mathbf{A}^{-1} is "the" matrix satisfying $\mathbf{A}\mathbf{A}^{-1} = \mathbf{I}_n$, but it is indeed the case that if a matrix has an inverse, the inverse is unique
- Some useful results:

$$(\mathbf{A} + \mathbf{B})^{\top} = \mathbf{A}^{\top} + \mathbf{B}^{\top}$$
 $(\mathbf{A}\mathbf{B})^{\top} = \mathbf{B}^{\top}\mathbf{A}^{\top}$
 $(\mathbf{A}\mathbf{B})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1}$
 $(\mathbf{A}^{\top})^{-1} = (\mathbf{A}^{-1})^{\top}$

Singular matrices

However, not all matrices have inverses; for example

$$\mathbf{A} = \left[\begin{array}{cc} 1 & 2 \\ 2 & 4 \end{array} \right]$$

- ullet There does not exist a matrix such that $\mathbf{A}\mathbf{A}^{-1}=\mathbf{I}_2$
- Such matrices are said to be singular
- Remark: Only square matrices have inverses; an $n \times m$ matrix ${\bf A}$ might, however, have a *left inverse* (satisfying ${\bf B}{\bf A}={\bf I}_m$) or *right inverse* (satisfying ${\bf A}{\bf B}={\bf I}_n$)

Positive definite

- A related notion is that of a "positive definite" matrix, which applies to symmetric matrices
- **Definition:** A symmetric $n \times n$ matrix \mathbf{A} is said to be positive definite if for all $\mathbf{x} \in \mathbb{R}^n$,

$$\mathbf{x}^{\mathsf{T}} \mathbf{A} \mathbf{x} > 0$$
 if $\mathbf{x} \neq 0$

- The two notions are related in the sense that if ${\bf A}$ is positive definite, then (a) ${\bf A}$ is not singular and (b) ${\bf A}^{-1}$ is also positive definite
- If $\mathbf{x}^{\top} \mathbf{A} \mathbf{x} \geq 0$, then \mathbf{A} is said to be positive semidefinite
- In statistics, these classifications are particularly important for variance-covariance matrices, which are always positive semidefinite (and positive definite, if they aren't singular)

Square root of a matrix

- These concepts are important with respect to knowing whether a matrix has a "square root"
- **Definition:** An $n \times n$ matrix A is said to have a *square root* if there exists a matrix B such that BB = A.
- Theorem: Let A be a positive definite matrix. Then there exists a unique matrix $A^{1/2}$ such that $A^{1/2}A^{1/2} = A$.
- Positive semidefinite matrices have square roots as well, although they aren't necessarily unique

Rank

- We also need to be familiar with the concept of matrix rank (there are many ways of defining rank; all are equivalent)
- **Definition:** The *rank* of a matrix is the dimension of its largest nonsingular submatrix.
- For example, the following 3×3 matrix is singular, but contains a nonsingular 2×2 submatrix, so its rank is 2:

$$\mathbf{A} = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 4 & 6 \\ 1 & 0 & 1 \end{bmatrix}$$

• Note that a nonsingular $n \times n$ matrix has rank n, and is said to be *full rank*

Rank and multiplication

- There are many results and theorems involving rank; we're not going to cover them all, but it is important to know that rank cannot be increased through the process of multiplication
- Theorem: For any matrices A and B with appropriate dimensions, $rank(AB) \le rank(A)$ and $rank(AB) \le rank(B)$.
- In particular, $rank(\mathbf{A}^{\top}\mathbf{A}) = rank(\mathbf{A}\mathbf{A}^{\top}) = rank(\mathbf{A})$.

Expectation and variance

- In addition, we need some results on expected values of vectors and functions of vectors
- First of all, we need to define expectation and variance as they pertain to random vectors
- **Definition:** Let $\mathbf{x} = (X_1 \ X_2 \ \cdots X_d)^{\top}$ denote a vector of random variables, then $\mathbb{E}(\mathbf{x}) = (\mathbb{E} X_1 \ \mathbb{E} X_2 \ \cdots \mathbb{E} X_d)^{\top}$. Meanwhile, $\mathbb{V}\mathbf{x}$ is a $d \times d$ matrix:

$$\mathbb{V}\mathbf{x} = \mathbb{E}\{(\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^{\top}\} \text{ with elements}$$
$$(\mathbb{V}\mathbf{x})_{ij} = \mathbb{E}\left\{(X_i - \mu_i)(X_j - \mu_j)\right\},$$

where $\mu_i = \mathbb{E}X_i$. The matrix $\mathbb{V}\mathbf{x}$ is referred to as the *variance-covariance matrix* of \mathbf{x} .

Linear and quadratic forms

• Letting ${\bf A}$ denote a matrix of constants and ${\bf x}$ a random vector with mean ${\boldsymbol \mu}$ and variance ${\boldsymbol \Sigma}$,

$$egin{aligned} \mathbb{E}(\mathbf{A}^{ op}\mathbf{x}) &= \mathbf{A}^{ op} oldsymbol{\mu} \ \mathbb{V}(\mathbf{A}^{ op}\mathbf{x}) &= \mathbf{A}^{ op} oldsymbol{\Sigma} \mathbf{A} \ \mathbb{E}(\mathbf{x}^{ op} \mathbf{A} \mathbf{x}) &= oldsymbol{\mu}^{ op} \mathbf{A} oldsymbol{\mu} + \mathrm{tr}(\mathbf{A} oldsymbol{\Sigma}), \end{aligned}$$

where $tr(\mathbf{A}) = \sum_{i} A_{ii}$ is the trace of \mathbf{A}

Some useful facts about traces:

$$\mathrm{tr}(\mathbf{A}\mathbf{B}) = \mathrm{tr}(\mathbf{B}\mathbf{A})$$
 $\mathrm{tr}(\mathbf{A} + \mathbf{B}) = \mathrm{tr}(\mathbf{A}) + \mathrm{tr}(\mathbf{B})$
 $\mathrm{tr}(c\mathbf{A}) = c\,\mathrm{tr}(\mathbf{A})$
 $\mathrm{tr}(\mathbf{A}) = \mathrm{rank}(\mathbf{A})$ if $\mathbf{A}\mathbf{A} = \mathbf{A}$

Eigendecompositions

- Finally, we'll also take a moment to introduce some facts about eigenvalues
- The most important thing about eigenvalues is that they allow us to "diagonalize" a matrix: if $\bf A$ is a symmetric $d\times d$ matrix, then it can be factored into:

$$\mathbf{A} = \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^{\mathsf{T}},$$

where Λ is a diagonal matrix containing the eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_d$ of $\mathbf A$ and the columns of $\mathbf Q$ are its eigenvectors

• Furthermore, eigenvectors are orthonormal, so we have $\mathbf{Q}^{\top}\mathbf{Q} = \mathbf{Q}\mathbf{Q}^{\top} = \mathbf{I}$

Eigenvalues and "size"

- This is very helpful from a conceptual standpoint, as it allows us to separate the "size" of a matrix (Λ) from its "direction(s)" (Q)
- For example, we have already seen that one measure of the size of a matrix is based on $\lambda_{\rm max}$ (for a symmetric matrix, its spectral norm is its largest eigenvalue)
- In addition, the trace and determinant, two other ways of quantifying the "size" of a matrix, are simple functions of the eigenvalues:

$$\circ \operatorname{tr}(\mathbf{A}) = \sum_{i} \lambda_{i}$$

$$\circ$$
 $|\mathbf{A}| = \prod_{i} \lambda_{i}$

Eigenvalues and inverses

- Once one has obtained the eigendecomposition of A, calculating its inverse is straightforward
- If \mathbf{A} is not singular, then $\mathbf{A}^{-1} = \mathbf{Q} \mathbf{\Lambda}^{-1} \mathbf{Q}^{\top}$; note that since $\mathbf{\Lambda}$ is diagonal, its inverse is trivial to calculate
- Even if ${\bf A}$ is singular, we can obtain something called a "generalized inverse": ${\bf A}^- = {\bf Q}{\bf \Lambda}^-{\bf Q}^\top$, where $({\bf \Lambda}^-)_{ii} = \lambda_i^{-1}$ if $\lambda_i \neq 0$ and $({\bf \Lambda}^-)_{ii} = 0$ otherwise
- Many other important properties of matrices can be deduced entirely from their eigenvalues:
 - A is positive definite if and only if $\lambda_i > 0$ for all i
 - A is positive semidefinite if and only if $\lambda_i \geq 0$ for all i
 - o If ${\bf A}$ has rank r, then ${\bf A}$ has r nonzero eigenvalues and the remaining d-r eigenvalues are zero

Extreme values

- Lastly, there is a connection between a matrix's eigenvalues and the extreme values of its quadratic form
- Let the eigenvalues $\lambda_1, \ldots, \lambda_d$ of $\mathbf A$ be ordered from largest to smallest. Over the set of all vectors $\mathbf x$ such that $\|\mathbf x\|_2 = 1$,

$$\max \mathbf{x}^{\mathsf{T}} \mathbf{A} \mathbf{x} = \lambda_1$$

and

$$\min \mathbf{x}^{\mathsf{T}} \mathbf{A} \mathbf{x} = \lambda_d$$