Adjoint Differentiation for generic matrix functions

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Abstract

We derive a formula for the adjoint $\overline{A}$ of a square-matrix operation of the form $C = f(A)$, where $f$ is holomorphic in the neighborhood of each eigenvalue. We then apply the formula to derive closed-form expressions in particular cases of interest such as the case when we have a spectral decomposition $A = UDU^{-1}$, the spectrum cut-off $C = A_+$ and the Nearest Correlation Matrix routine. Finally, we explain how to simplify the computation of adjoints for regularized linear regression coefficients.

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1 Introduction

This paper gives a general approach to calculating adjoints of functions $f(A)$ of square matrices. We complement the works of M.Giles [1] and B.N.Huge [8], where they provide a list of closed-form formulas for adjoints of some useful matrix operations.

It is important to emphasize that we do not require the eigenvalues $\lambda_i \in \text{Sp}(A)$ to be distinct and can apply the approach even when $A$ does not admit a spectral decomposition $A = UDU^{-1}$ by using more general normal form decompositions (e.g. Schur or Jordan). However, we do require the decomposition to keep the identity matrix invariant. For instance, if $A$ is not symmetric, we can’t use the singular value decomposition (SVD) $A = UDV^T$ since $UV^T \neq Id$.

By the Cauchy’s formulas we have

$$f(z) = -\frac{1}{2\pi i} \int_{\Gamma} \frac{f(\lambda)}{z - \lambda} d\lambda, \quad f'(z) = \frac{1}{2\pi i} \int_{\Gamma} \frac{f(\lambda)}{(z - \lambda)^2} d\lambda,$$

where $f$ is holomorphic on an open set containing $z$ and $\Gamma$ is the boundary of that set. These formulas will be crucial for calculating elements of the adjoint.

To derive the general formula for $\overline{A}$ we shall use the following generalization:

$$f(A) = -\frac{1}{2\pi i} \int_{\Gamma} f(\lambda) \text{Res}(\lambda) d\lambda, \quad \text{Res}(\lambda) = (A - \lambda I)^{-1},$$

where $f$ is holomorphic on an open set containing $\text{Sp}(A)$, and $\Gamma$ is the boundary of that set. Note that we don’t require the set to be connected so a union of disjoint discs around $\lambda_i \in \text{Sp}(A)$ works. We refer to [2], [4] for the proof.

Notation. Matrices in what follows are real-valued of size $n \times n$ unless stated otherwise. We use the standard notations $X^{-T} = (X^{-1})^T = (X^T)^{-1}$ for the transpose of the inverse matrix of $X$, $X_{ij}$ for the $ij$ element of $X$ and $E_{ij}$ for the matrix with 1 in the $ij$ position and zeroes elsewhere. We denote by $X.\text{row}(i)$ the $i$-th row of $X$ and by $X.\text{col}(j)$ the $j$-th column of $X$. We also denote by $A \circ B$ the component-wise (Hadamard) product $(A \circ B)_{ij} = A_{ij}B_{ij}$ of square matrices $A$ and $B$ of the same size.

2 The general formula for $\overline{A}$

We first calculate the partial derivative $f'_{ij}(A)$ of $f(A)$ with respect to $A_{ij}$. Note that for $\lambda \notin \text{Sp}(A)$ and $\varepsilon \to 0$ we have

$$(A - \lambda + \varepsilon E_{ij})^{-1} = [(A - \lambda)(I + \text{Res}(\lambda)\varepsilon E_{ij})]^{-1} = [I - \text{Res}(\lambda)\varepsilon E_{ij} + O(\varepsilon^2)] \text{Res}(\lambda)$$

\footnote{Note that a square matrix $A$ defines a linear operator $A : V \to V$ on a finite dimensional space $V$. The proof in the references works for a general class of linear operators, including the finite dimensional case.}
and so
\[ \text{Res}(\lambda)_{ij}' = -\text{Res}(\lambda)E_{ij}\text{Res}(\lambda). \]
Differentiating (2) with respect to \( A_{ij} \) gives
\[ f'_{ij}(A) = -\frac{1}{2\pi i} \int_{\Gamma} f(\lambda)\text{Res}(\lambda)_{ij}' d\lambda = \frac{1}{2\pi i} \int_{\Gamma} f(\lambda)\text{Res}(\lambda)E_{ij}\text{Res}(\lambda) d\lambda, \]
where we can take \( \Gamma \) to be a set of small circles around each \( \lambda_i \in \text{Sp}(A) \) (since \( f \) is holomorphic in the neighborhood each eigenvalue).

Following [1], we can now calculate elements \( \overline{A}_{ij} \) of the adjoint \( \overline{A} \):
\[ \overline{A}_{ij} = \sum_{k,l} \left[ f'_{ij}(A) \right]_{k,l} \left[ f(A) \right]_{k,l} = \text{Tr} \left( f'_{ij}(A) \overline{f(A)}^T \right) = \frac{1}{2\pi i} \int_{\Gamma} f(\lambda) \text{Tr} \left( \text{Res}(\lambda)E_{ij}\text{Res}(\lambda)\overline{f(A)}^T \right) d\lambda = \frac{1}{2\pi i} \int_{\Gamma} f(\lambda) \text{Tr} \left( E_{ij}\text{Res}(\lambda)\overline{f(A)}^T \text{Res}(\lambda) \right) d\lambda. \]
Since for any matrix \( M \) one has \( \text{Tr}(E_{ij}M) = M_{ji} \), we get a general formula for \( \overline{A} \):
\[ \overline{A} = \frac{1}{2\pi i} \int_{\Gamma} f(\lambda) \text{Res}^T(\lambda)\overline{f(A)}\text{Res}(\lambda)d\lambda \] (3)

Now to obtain a closed-form expression for \( \overline{A} \) it remains to transform \( \text{Res}(\lambda) \) to an appropriate (keeping the identity matrix invariant) normal form and collect residues. We shall perform this computation in some cases of interest.

3 Special cases

3.1 Spectral decomposition \( A = UDU^{-1} \):
Suppose that our matrix has a spectral decomposition \( A = UDU^{-1} \) (including the case when not all the eigenvalues are distinct). Then \( \text{Res}(\lambda) = U(D - \lambda I)^{-1}U^{-1} \) gives a (spectral) decomposition of \( \text{Res}(\lambda) \).

It is easy to see from [1] that:
\[ \frac{1}{2\pi i} \int_{\Gamma} \frac{f(\lambda)d\lambda}{(\lambda - \lambda_i)(\lambda - \lambda_j)} = \begin{cases} f'(\lambda_i), & \lambda_i = \lambda_j \\ \frac{f(\lambda_i) - f(\lambda_j)}{\lambda_i - \lambda_j}, & \lambda_i \neq \lambda_j \end{cases} \] (4)
Let \( F \) be a matrix with these values:
\[ F_{ij} = \begin{cases} f'(\lambda_i), & \lambda_i = \lambda_j \\ \frac{f(\lambda_i) - f(\lambda_j)}{\lambda_i - \lambda_j}, & \lambda_i \neq \lambda_j \end{cases} \] (5)
Substituting \( \text{Res}(\lambda) = U(D - \lambda I)^{-1}U^{-1} \) into (3) and applying (4) we see that
\[
\overline{A}^T = U \left( F \circ (U^{-1}f(A)^T U) \right) U^{-1}.
\]

We want to stress here that \( \overline{A} \) is expressed directly in terms of \( \overline{f(A)} \) and there is no need to calculate adjoints to matrix decomposition components \( U \) and \( D \).

### 3.2 Spectrum cut-off

Suppose now that \( A \) is symmetric and \( f(A) = A_+ \) is the projector on the positive spectrum. Then we may integrate over a contour \( \Gamma^+ \) enclosing only the positive eigenvalues instead of integrating over \( \Gamma \) (this follows from the Riesz decomposition theorem for operators, see e.g. [3], [5]). Using the decomposition \( A = UDU^T \) we immediately get
\[
\overline{A} = U \left( F \circ (U^T \overline{A}_+ U) \right) U^T
\]
with
\[
F_{ij} = \begin{cases} 
\text{sgn}(\lambda_i), & \lambda_i = \lambda_j \\
\max(\lambda_i, 0) - \max(\lambda_j, 0), & \lambda_i \neq \lambda_j 
\end{cases} \frac{\lambda_i - \lambda_j}{\lambda_i - \lambda_j},
\]
\[
\lambda_i \neq \lambda_j
\]

Note that (6) can be generalized to other \( f(A) \), as we will see later.

For smoothing purposes it is reasonable to use a smoothed indicator function \( f(A) = \frac{1}{2} \left( I + \tanh \left( \frac{A}{\delta} \right) \right) \) instead of \( f(A) = A_+ \). In that case one should use (5) to define \( F \).

### 4 Nearest Correlation Matrix

#### 4.1 Setup

Let \( A \in \mathbb{R}^{n \times n} \) be a fixed symmetric matrix. Recall that the Nearest Correlation Matrix (NCM) is the solution \( X \) to the following minimization problem:
\[
\min \left\{ \|A - X\|_F, : X = X^T, X \geq 0, \text{Diag}(X) = e \right\}.
\]
Here \( \| \cdot \|_F \) is the Frobenius norm, \( \text{Diag}(X) \) is the vector of diagonal elements of \( X \), \( e = \text{Diag}(Id) \) is the vector of 1-s. By \( X \geq 0 \) we mean that any \( \lambda \in \text{Sp}(X) \) satisfies \( \lambda \geq 0 \) (the matrix is positive semidefinite).

Let \( C = \text{NCM}(A) \) be the Nearest Correlation Matrix. Then it is known that
\[
C = (A + \text{diag}(y_*))_+,
\]
where \( y_* = y_*(A) \) is a solution to the minimization problem
\[
\min_{y \in \mathbb{R}^n} \left( \frac{1}{2} \| (A + \text{diag}(y))_+ \|_F^2 - e^T y \right).
\]

Here, \( \text{diag}(y) \), \( y \in \mathbb{R}^n \) is the diagonal matrix with values on the diagonal coming from \( y \) (so that we have \( \text{Diag}(\text{diag}(y)) = y \)). See [6] for the proof of this result.
4.2 Calculation

Using results from section 3.2 we will show that

\[ \overline{A} = \overline{A}_1 + \overline{A}_2, \]

where

\[ \overline{A}_2 = V \left( F \circ (V^T \overline{C} V) \right) V^T \]

and

\[ \overline{A}_1 = -V \left( F \circ (V^T \text{ diag } (J^{-T} \text{ Diag}(\overline{A}_2)) V) \right) V^T. \]

Here \( V \) and \( F \) are defined similarly to \( U \) and \( F \) respectively in (6), (7) but for the operation \((A + \text{ diag}(y^*_+))_+\). These matrices are usually known at the forward pass, namely, at the last iteration of the Newton method for the minimization problem (8).

The matrix \( J = \{J_{ij}\} \) is given by

\[ J_{ij} = V \cdot \text{row}(i) T^{ij} V^T \cdot \text{col}(j), \]

where \( T^{ij} = \{[T^{ij}]_{kl}\} \) has elements

\[ [T^{ij}]_{kl} = V_{ik} V_{il} F_{kl}. \]

**Proof.** The NCM routine consists of finding the solution \( y_+ = y_+(A) \) of (8) that also solves \( M(y) = e \), where

\[ M(y) = \text{Diag}(A + \text{ diag}(y))_+. \]

Then \( C = \text{NCM}(A) = (A + \text{ diag}(y_+))_+ \). So for the adjoint we have:

\[ \overline{A} = \overline{A}_1 + \overline{A}_2, \]

where

\[ \overline{A}_2 = V \left( F \circ (V^T \overline{C} V) \right) V^T \]

Now we have to backpropagate through the solver which is straightforward if we set the correct adjoint values before it starts (see e.g. [7], (19),(20)). Namely, suppose that we have the solver backpropogate an implicit function \( x = x(c) \) by equation \( M(x, c) = 0 \). Then we should set \( \overline{M} = -J^{-T} \overline{\pi} \) (where \( J \) is the Jacobian) before backpropagating.

In our situation, a straightforward calculation using formula (6) gives the \( J \) above and setting \( \overline{M} = -J^{-T} \text{ Diag}(\overline{A}_2) \) we get

\[ \overline{A}_1 = V \left( F \circ (V^T \text{ diag}(\overline{M}) V) \right) V^T. \]

\[ ^2 \text{Another representation can be found in [6].} \]
5 Regression Regularization

5.1 Setup

Given a matrix $B$ of dimension $m \times k$ and a matrix $A$ of dimension $n \times m$, the standard formula for regression coefficients is

$$\beta = (AA^T)^{-1} AB.$$ 

In [8] B.N.Huge suggests computing regression coefficients $\beta$ using spectrum cut-off with a spectrum threshold $\varepsilon \geq 0$ and a Tikhonov regularization parameter $\lambda \geq 0$:

$$\beta = (AA^T)^{-1,\varepsilon,\lambda} AB,$$

where for a positive semidefinite symmetric matrix $M = UDU^T$ we define $M^{-1}_{\varepsilon,\lambda}$ by

$$M^{-1}_{\varepsilon,\lambda} = U \text{diag} \left( \frac{\text{sgn}(\lambda_i - \varepsilon)}{\lambda_i + \lambda} \right) U^T.$$ 

Later in [9] this approach has been used by B.N.Huge and A.Savine to calculate stable adjoints for Callable Exotics prices.

5.2 Calculation

We only compute the adjoints for $M^{-1}_{\varepsilon,\lambda}$ since other operations in [9] are matrix multiplications and corresponding formulas for adjoints are simple and well-known (see [1], [8]).

In [8] the author obtains adjoints of (9) by calculating adjoints for elements of the SVD decomposition of the matrix $A$. We trust that our approach is easier to verify and the final expression is shorter than the formula [8, (6)].

Indeed, (6) generalizes to give the required expression for adjoints

$$\overline{M} = U \left( F \circ (U^T M^{-1}_{\varepsilon,\lambda} U) \right) U^T,$$

where

$$F_{ij} = \begin{cases} -\text{sgn}(\lambda_i - \varepsilon), & \lambda_i = \lambda_j \\ \left( \frac{\text{sgn}(\lambda_i - \varepsilon)}{\lambda_i + \lambda} - \frac{\text{sgn}(\lambda_j - \varepsilon)}{\lambda_j + \lambda} \right) \frac{1}{\lambda_i - \lambda_j}, & \lambda_i \neq \lambda_j \end{cases}.$$ 

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