Some Remarks on Computing Gradients of a Matrix Exponential

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1 The Dynamical Systems View

We are interested in computing

$$\nabla_J \exp(tQ) = \lim_{\epsilon \to 0} \frac{\exp(t(Q + \epsilon J) - \exp(tQ)}{\epsilon} \tag{1.1}$$

–eq:grad:def˝

matrices $J, Q \in \mathbb{R}^{d \times d}$. Noting that $X(t) := \exp(tQ)$ obeys the (matrix valued) ordinary differential equation

$$\frac{dX}{dt} = QX, \quad X(0) = I, \tag{1.2}$$

–eq:exptQ˝

and taking $X^\epsilon = \exp(tQ + \epsilon J)$, $Y^\epsilon = \epsilon^{-1}(X^\epsilon - X)$ we have

$$\frac{dY^\epsilon}{dt} = QY^\epsilon + JX^\epsilon, \quad Y^\epsilon(0) = 0.$$

Hence taking a limit as $\epsilon \to 0$ we find that $Y = \nabla_J \exp(tQ)$ obeys

$$\frac{dY}{dt} = QY + JX, \quad Y^\epsilon(0) = 0, \tag{1.3}$$

–eq:sen:eq˝

and so variation of constants yields that, for any $t \geq 0$,

$$Y(t) = \exp(tQ) \int_0^t \exp(-sQ) J \exp(sQ) ds = \exp(tQ) \sum_{k,m=0}^{\infty} \int_0^t \frac{(-s)^k Q^k J s^m Q^m}{k! m!} ds \tag{1.4}$$

–eq:var:const:1˝

$$= \exp(tQ) \sum_{k,m=0}^{\infty} (-1)^k \frac{Q^k J Q^m}{m! k! (m + k + 1)} t^{k+m+1} = \exp(tQ) \sum_{k,m=0}^{\infty} (-1)^k \frac{(m+k)!}{m! k!} \frac{Q^k J Q^m}{(m + k + 1)!} t^{k+m+1}$$

$$= \exp(tQ) \sum_{n=0}^{\infty} \frac{t^{n+1}}{(n+1)!} \left(\sum_{l=0}^{n} (-1)^l \binom{n}{l} Q^l J Q^{n-l} \right) \tag{1.5}$$

–eq:var:const:2˝

Note that the last line corresponds to the identity from [NH95]. Taking the first order approximation in (1.5) gives

$$\tilde{\nabla}_J \exp(tQ) = t \exp(tQ) J, \tag{1.6}$$

which we see from (1.4) is evidently exact in the case when J and Q commute.

Next notice that if we differentiate $\tilde{Y} = t \exp(tQ) J$ we find that $\tilde{Y}$ obeys

$$\frac{d\tilde{Y}}{dt} = Q\tilde{Y} + \exp(tQ) J, \quad \tilde{Y}(0) = 0. \tag{1.7}$$

Taking

$$Z(t) = Y(t) - \tilde{Y}(t) = \nabla_J \exp(tQ) - t \exp(tQ) J \tag{1.8}$$

–eq:true:diff˝

and comparing with (1.3) yields

$$\frac{dZ}{dt} = QZ + J\exp(tQ) - \exp(tQ)J, \quad Z(0) = 0. \tag{1.9}$$

eq:Z:dym

and hence

$$Z(t) = \exp(tQ)\int_0^t (\exp(-sQ)J\exp(sQ) - J)ds = \exp(tQ)\sum_{n=1}^{\infty}\frac{t^{n+1}}{(n+1)!}\left(\sum_{l=0}^{n}(-1)^l\binom{n}{l}Q^l J Q^{n-l}\right) \tag{1.10}$$

eq:ass:procs

as could also be directly deduced from (1.4), (1.5).

2 Time Asymptotic Approximation Error

We would like to deduce the time asymptotic behavior of $Z(t) := \nabla_J \exp(tQ) - t\exp(tQ)J$. Evidently we need some further structure for Q. Consider the class of (irreducible) rate matrices

$$\mathcal{R} = \{Q \in \mathbb{R}^{d\times d} | Q_{i,j} > 0 \text{ for } j \neq i \text{ and } \sum_{j=1}^{d} Q_{i,j} = 0 \text{ for each } i\} \tag{2.1}$$

and subclass of diagonalizable matrices

$$\begin{aligned}\mathcal{D} = \{Q \in \mathcal{R} | Q &\text{ is diagonalizable and for a suitable diagonalizing matrix } M, D = MQM^{-1}\\ &\Re D_{i,i} < 0, \text{ for } i = 1, \dots, d-1, D_{d,d} = 0\}.\end{aligned} \tag{2.2}$$

eq:Q:spc

Notice that, for $Q \in \mathcal{D}$,

$$Q\exp(tQ) = M^{-1}DMM^{-1}\exp(tD)M = M^{-1}D\exp(tD)M$$

and hence

$$\|Qe^{tQ}\| \leq \|M^{-1}\|\|M\|\left(\sum_{j=1}^{d-1}|D_{i,i}\exp(tD_{i,i})|^2\right)^{1/2} \leq \sqrt{d-1}\|M^{-1}\|\|M\|e_m\exp(-te_M) \tag{2.3}$$

eq:decay:est:1

where here and below $\|\cdot\|$ denotes the standard Frobenius norm on $\mathbb{C}^{d\times d}$ and

$$e_m = \min_{i=1,\dots,d-1}|D_{i,i}|, \quad e_M = \max_{i=1,\dots,d-1}|D_{i,i}|. \tag{2.4}$$

eq:max:min:D

Thus $\|Qe^{tQ}\|$ decays with an exponential rate and so with (1.2) so does de^{-tQ}/dt

Building on this observation and (1.10) we might expect, for t large, that

$$Z(t) \approx \exp(tQ)J\sum_{n=1}^{\infty}\frac{t^{n+1}Q^n}{(n+1)!} = \exp(tQ)JQ^+\sum_{n=1}^{\infty}\frac{t^{n+1}Q^{n+1}}{(n+1)!} = \exp(tQ)JQ^+(\exp(tQ) - I - tQ) \tag{2.5}$$

$$\approx -\exp(tQ)JQ^+(I + tQ) \tag{2.6}$$

eq:ass:procs:der

where Q^+ is the pseudo-inverse Q. Notice that

$$\tilde{Z}(t) := -\exp(tQ)JQ^+(I + tQ) \tag{2.7}$$

eq:t:ass:diff

obeys

$$\frac{d\tilde{Z}}{dt} = Q\tilde{Z} - \exp(tQ)JQ^+Q, \quad \tilde{Z}(0) = -JQ^+. \tag{2.8}$$

eq:tZ:dym

Here in our heuristic (2.6) we used our structural assumptions on $Q \in \mathcal{D}$ to infer that

$$Q = QQ^+Q = Q^+Q^2.$$

To justify dropping $\exp(tQ)JQ^+e^{tQ}$ as small for large t we observe analogously to (2.3)

$$\|Q^+e^{tQ}\| \leq \|M^{-1}\|\|M\| \left(\sum_{j=1}^{d-1} |D_{i,i}^{-1} \exp(tD_{i,i})|^2 \right)^{1/2} \leq \sqrt{d-1}\|M^{-1}\|\|M\| e_M^{-1} \exp(-te_M). \tag{2.9}$$ ~eq:decay:est:2~

with e_M defined as in (2.4).

Let us now prove that indeed $-\exp(tQ)JQ^+(I+tQ) \approx \nabla_J \exp(tQ) - t\exp(tQ)J$ with an error decaying at an exponential rate as $t \to \infty$. More precisely we have the following

thm:ass:error **Theorem 2.1.** *For any $Q \in \mathcal{D}$ and any $J \in \mathbb{C}^{d\times d}$*

$$\| -\exp(tQ)JQ^+(I+tQ) + Q^+J(I-QQ^+) - (\nabla_J \exp(tQ) - t\exp(tQ)J)\| \leq Ce^{-\kappa t} \tag{2.10}$$

for constants $C, \kappa > 0$ depending on Q and J explicitly as

$$C := \quad \kappa := \tag{2.11}$$

Proof. Take $W(t) = \tilde{Z}(t) - Z(t)$ where are defined as in (2.7), (1.8) respectively. Notice that W follows the dynamic, cf. (1.9), (2.8)

$$\frac{dW}{dt} = QW + \exp(tQ)J(I - Q^+Q) - J\exp(tQ) \quad W(0) = -JQ^+ \tag{2.12}$$ ~eq:ass:err:eq~

With variation of constants we arrive at the expression

$$W(t) = -\exp(tQ) \left(JQ^+ + \int_0^t (\exp(-sQ)J\exp(sQ) - J(I-Q^+Q))ds \right) \tag{2.13}$$ ~eq:ass:err:sol~

But we observe the following for expression inside of the integral

$$\begin{aligned}
&\exp(-sQ)J\exp(sQ) - J(I-Q^+Q)\\
&\quad= \exp(-sQ)QQ^+J\exp(sQ) + \exp(-sQ)(I-QQ^+)J\exp(sQ) - J(I-Q^+Q)\\
&\quad= \exp(-sQ)QQ^+J\exp(sQ) + (I-QQ^+)J\exp(sQ) - J(I-Q^+Q)\\
&\quad= \exp(-sQ)QQ^+J\exp(sQ) + (I-QQ^+)JQQ^+\exp(sQ)\\
&\qquad + (I-QQ^+)J(I-QQ^+)\exp(sQ) - J(I-Q^+Q))\\
&\quad= \exp(-sQ)QQ^+J\exp(sQ) + (I-QQ^+)JQQ^+\exp(sQ)\\
&\qquad + (I-QQ^+)J(I-QQ^+) - J(I-Q^+Q))\\
&\quad= \exp(-sQ)QQ^+J\exp(sQ) + (I-QQ^+)JQQ^+\exp(sQ) - QQ^+J(I-QQ^+)\\
&\quad= \exp(-sQ)QQ^+JQQ^+\exp(sQ) + \exp(-sQ)QQ^+J(I-QQ^+)\\
&\qquad + (I-QQ^+)JQQ^+\exp(sQ) - QQ^+J(I-QQ^+)
\end{aligned}$$

In deriving the above identity we have repeatedly used that

$$\begin{aligned}
(I-QQ^+)\exp(sQ) &= M^{-1}M(I-QQ^+)\exp(sQ)M^{-1}M = M^{-1}M(I-QQ^+)M^{-1}M\exp(sQ)M^{-1}M\\
&= M^{-1}(I-DD^+)\exp(sD)M = I - QQ^+
\end{aligned}$$

Hence combining the above we find

$$\begin{aligned}
W(t) =& -\exp(tQ)\left(JQ^+ + \int_0^t (I-QQ^+)JQQ^+\exp(sQ) + \exp(-sQ)QQ^+J(I-QQ^+))ds \right)\\
&- \int_0^t \exp((t-s)Q)Q^+QJQ^+Q\exp(sQ)ds + t\exp(tQ)Q^+QJ(I-QQ^+)\\
:=& T_1(t) + T_2(t) + T_3(t)
\end{aligned}$$

Regarding $T_1(t)$ observe that

$$\begin{aligned}
T_1(t) &= -\exp(tQ)\Big(JQ^+ + \int_0^t (I-QQ^+)JQQ^+\exp(sQ) + \exp(-sQ)QQ^+J(I-QQ^+))ds\Big)\\
&= -\exp(tQ)\Big(JQ^+ + \int_0^t \frac{d}{ds}[(I-QQ^+)JQ^+\exp(sQ) - \exp(-sQ)Q^+J(I-QQ^+)]ds\Big)\\
&= -\exp(tQ)\Big(JQ^+ + (I-QQ^+)JQ^+\exp(tQ) - \exp(-tQ)Q^+J(I-QQ^+)\\
&\qquad - (I-QQ^+)JQ^+ + Q^+J(I-QQ^+)\Big)\\
&= -\exp(tQ)\Big(QQ^+JQ^+ + (I-QQ^+)JQ^+\exp(tQ) + Q^+J(I-QQ^+)\Big) - Q^+J(I-QQ^+)
\end{aligned}$$

Turning to $T_2(t)$ and letting $\bar{J} = M^{-1}JM$ and I_{-d} be the identity matrix with final diagonal element set to 0, we have

$$\begin{aligned}
T_2(t) &= \int_0^t \exp((t-s)Q)Q^+QJQ^+Q\exp(sQ)ds\\
&= M\left(\int_0^t (\exp((t-s)D)I_{-d})\bar{J}(I_{-d}\exp(sD))ds\right)M^{-1}\\
&= M\left(\int_0^t \bar{J}\circ\Psi(t,s)ds\right)M^{-1} = M\left(\bar{J}\circ\int_0^t \Psi(t,s)ds\right)M^{-1}\\
&= M\left(\bar{J}\circ\Phi(t)\right)M^{-1}
\end{aligned}$$

where the elements of $\Psi(t,s)$ satisfy

$$\Psi_{ij}(t,s) = \begin{cases} e^{(t-s)D_{j,j}+sD_{i,i}}, & i,j<d,\ i\neq j\\ e^{tD_{j,j}}, & i,j<d,\ i=j\\ 0, & o/w \end{cases},$$

and

$$\Phi_{ij}(t) = \int_0^t \Psi_{ij}(t,s)ds = \begin{cases} \frac{e^{tD_{i,i}}-e^{tD_{j,j}}}{D_{i,i}-D_{j,j}}, & i,j<d,\ i\neq j\\ te^{tD_{j,j}}, & i,j<d,\ i=j\\ 0, & o/w \end{cases}.$$

Then, by the definition of the Frobenius norm

$$\begin{aligned}
\|T_2(t)\| &= \|M\left(\bar{J}\circ\Phi(t)\right)M^{-1}\| \le \|\bar{J}\circ\Phi(t)\|\|M\|\|M^{-1}\|\\
&= \left(\sum_{i,j}|\bar{J}_{ij}|^2|\Phi_{ij}(t)|^2\right)^{1/2}\|M\|\|M^{-1}\|\\
&\le \left(\sum_{i,j}|\Phi_{ij}(t)|^4\right)^{1/4}\left(\sum_{i,j}|\bar{J}_{ij}|^4\right)^{1/4}\|M\|\|M^{-1}\|\\
&\le \left((D-1)^2\max_{i,j}|\Phi_{ij}(t)|^4\right)^{1/4}\|\bar{J}^{\circ 2}\|^{1/2}\|M\|\|M^{-1}\|\\
&= \left(\max_{i,j}|\Phi_{ij}(t)|\right)\sqrt{D-1}\|\bar{J}^{\circ 2}\|^{1/2}\|M\|\|M^{-1}\|.
\end{aligned}$$

Since $\max|\Phi_{ij}|$ goes to 0 at an exponential rate, we have $\|T_2(t)\|\to 0$ as $t\to\infty$. Finally,

$$\begin{aligned}
\|T_3(t)\| &= \|t\exp(tQ)Q^+QJ(I-QQ^+)\|\\
&\le \left(t\max_{i<d}e^{tD_{i,i}}\right)\|J\|\|\|M\|^2\|M^{-1}\|^2.
\end{aligned}$$

[FINISH] $\square$

Get angle between

3 High-dimensional Asymptotics

Given the above result, it would be interesting to characterize the behavior of

$$\begin{aligned}\|Q^+J(I-QQ^+)\|_F &\leq \|M^{-1}D^+M\|_F\|J\|_F\|O^T(I-I_{-d})O\|_F\\ &\leq \|D^+\|_F\|M\|_F\|M^{-1}\|_F\|J\|_F\\ &= \frac{1}{e_m}\|M\|_F\|M^{-1}\|_F\|J\|_F\end{aligned}$$

for random Q as $d \to \infty$. Here, O is the orthogonal matrix obtained by diagonalizing QQ^+, and we have used the rotation invariance of the Frobenius norm. We are therefore interested in the complex modulus of the non-zero eigenvalue closest to the origin on the complex plain.

Questions/Comments:

- Empirically, $e_m \to \infty$ as $d \to \infty$.

4 Questions, Comments and Clarifications

(i) Where does the extra correction term $-Q^+J(I-QQ^+)$ come from?

(ii) $\mathcal{D}$ defined as (2.2) where Q lives is not a linear space? How does HMC work here? What is the underlying target distribution on $\mathcal{D}$?

(iii) How does the surrogate trajectory method implied by $\tilde{\nabla}_J \exp(tQ) = t\exp(tQ)J$ perform relative to e.g. an adjoint method which exactly computes $\nabla_J \exp(tQ)$?

(iv) Why not use a 'higher order' approximation of $\nabla_J \exp(tQ)$? For example we could take

$$\nabla_J \exp(tQ) \approx \exp(tQ)\int_0^t (I-sQ)J(I+sQ)ds = \exp(tQ)\left(tJ + \frac{t^2}{2}(JQ-QJ) - \frac{t^3}{3}QJQ\right). \quad (4.1)$$

Why is this a big deal to compute?

(v) Maybe we should try to prove a higher order version of (2.1) in any case.

(vi) The formula (1.5), (1.4) may be useful for developing surrogate trajectory methods for other Matrix coefficient estimation problems.

4.1 Estimation Problem 1: Determining the 'Potential' in a Toy QM Model.

Suppose we observe (some component of) $x(t) \in \mathbb{C}^d$ from the solution of

$$\frac{dx}{dt} = Ax, \quad x(0) = x_0, \quad (4.2)$$

where $A \in \{A \in \mathbb{C}^{d\times d} | A^* = -A\}$. If $|x_0| = 1$ then $|x(t)|$ can be interpreted as a discrete probability distribution on $\{1,\dots,d\}$ for any $t \geq 0$.

4.2 Estimation Problem 2: Back to the Advection Diffusion model.

Consider the advection-diffusion model

$$\partial_t \theta = (\kappa \Delta - \mathbf{u} \cdot \nabla)\theta \quad \theta(0) = \theta_0 \tag{4.3}$$

Denote

$$S_{\mathbf{u}}(t)\theta_0 := \theta(t; \theta_0, \mathbf{u}). \tag{4.4}$$

Then taking

$$\rho = \nabla_{\mathbf{v}} S_{\mathbf{u}}(t)\theta_0 := \lim_{\epsilon \to 0} \epsilon^{-1}(S_{\mathbf{u}+\epsilon\mathbf{v}}(t)\theta_0 - S_{\mathbf{u}}(t)\theta_0) \tag{4.5}$$

we have the ρ obeys

$$\partial_t \rho = (\kappa \Delta - \mathbf{u} \cdot \nabla) + \mathbf{v} \cdot \nabla\theta \quad \rho(0) = 0. \tag{4.6}$$

Here we still have the variation of constants formula

$$\rho(t) = \int_0^t S_{\mathbf{u}}(t-s)\mathbf{v} \cdot \nabla\theta(s)ds = \int_0^t S_{\mathbf{u}}(t-s)\mathbf{v} \cdot \nabla S_{\mathbf{u}}(s)\theta_0 ds. \tag{4.7}$$

References

ajfeld1995derivatives [NH95] Igor Najfeld and Timothy F Havel. Derivatives of the matrix exponential and their computation. *Advances in applied mathematics*, 16(3):321–375, 1995.