A Appendix

We now provide additional details for our results in Section 2 of the paper.

Lemma 1. Let A, B be full column rank matrices of size $n \times d$, with $\log(n) = d^{o(1)}$. Let S be an SRHT with $1 = \tilde{O}((d + \log(1/\delta))/\epsilon^2)$ rows. For any matrix B of size $n \times d$ we have

$$||X||_2 = ||(SA)^{\dagger}SB||_2 \lesssim ||A^{\dagger}B||_2 + \epsilon ||\Sigma^{-1}||_2 (\sqrt{(1+d/k)(||B||_2^2 + ||B||_F^2/k)}),$$

with probability 1 - 1/poly(d).

Proof. From Equation 5 in the body and the triangle inequality, we have

$$(SA)^{\dagger}SB = V\Sigma^{-1}(\sum_{k=0}^{\infty} T^{K})U^{\mathsf{T}}S^{\mathsf{T}}SB$$
(1)

$$\|(SA)^{\dagger}SB\|_{2} \le \|A^{\dagger}B\|_{2} + \|(SA)^{\dagger}SB - A^{\dagger}B\|_{2} \tag{2}$$

$$\leq \|A^{\dagger}B\|_{2} + \|V\Sigma^{-1}(\sum_{k=0}^{\infty} T^{k})U^{\mathsf{T}}S^{\mathsf{T}}SB - V\Sigma^{-1}U^{\mathsf{T}}B\|_{2}$$
(3)

$$\leq \|A^{\dagger}B\|_{2} + \|\Sigma^{-1}\|_{2} \sum_{k=0}^{\infty} \epsilon^{k} \|U^{\mathsf{T}}S^{\mathsf{T}}SB - U^{\mathsf{T}}B\|_{2} \tag{4}$$

$$\leq \|A^{\dagger}B\|_{2} + \|\Sigma^{-1}\|_{2} \frac{\epsilon}{1-\epsilon} \sqrt{(1+d/k)(\|B\|_{2}^{2} + \|B\|_{F}^{2}/k)} \tag{5}$$

where we used equation 8 in the body in the last step.

A.1 AD

Let us manually derive the AD for the least squares regression problem.

LLS(
$$A, b$$
) = LS($A^{T}A, A^{T}b$)
= LS(M, m)
(M, m) $\equiv (A^{T}A, A^{T}b)$
 $B = A^{T}$
(B_{1}, B_{2}) = (B, B)
 $C = B_{1}A$
 $d = B_{2}b$
 $\bar{A}_{M} = A\bar{M} + A\bar{M}^{T}$
 $\bar{A}_{m} = b\bar{m}^{T}$
 $\bar{A} = \bar{A}_{M} + \bar{A}_{m}$
= $A\bar{M} + A\bar{M}^{T} + b\bar{m}^{T}$
 $\bar{b} = A\bar{m}$
(\bar{M}, \bar{m}) = $\mathcal{J}^{T}(LS)(M, m)(\bar{y})$
= $(-\bar{m}y^{T}, LS(M^{T}, \bar{y}))$
= $(-LS(A^{T}A, \bar{y})y^{T}, LS(A^{T}A, \bar{y}))$

This gives us the final reverse mode AD:

$$\bar{A} = -A(A^{T}A)^{-1}\bar{y}y^{T}) - Ay\bar{y}^{T}(A^{T}A)^{-1} + by^{T}(A^{T}A)^{-1}$$
(6)

$$\bar{b} = A(A^{\mathrm{T}}A)^{-1}\bar{y} \tag{7}$$

¹For a function f, we use the notation $\tilde{O}(f)$ to denote $f \cdot \text{polylog}(f)$.

A.2 Approximation bounds

Let us derive some additional bounds which were missing in the main paper:

$$||Ay\bar{y}^{T}M^{-1} - Ay_D\bar{y}^{T}M_S^{-1}||_F \leq ||Ay\bar{y}^{T}M^{-1} - Ay_D\bar{y}^{T}M^{-1}||_F + ||Ay_D\bar{y}^{T}(M - M_S^{-1})||_F$$

$$\leq ||U(I - (U^{T}S^{T}SU)^{-1})U^{T}b||_F + \epsilon ||Ay_D|| ||\bar{y}|| ||\Sigma^{-1}||_2 ||\Sigma^{-1}||_F$$

$$\leq \epsilon (||b||_2 + ||b||_2 ||\bar{y}||_2 ||\Sigma^{-1}||_2 ||\Sigma^{-1}||_F)$$

$$(10)$$

Table 1: Cheat sheet to derive AD.

Original	Forward Transform	Reverse Transform
z = a + b	$\dot{z} = \dot{a} + \dot{b}$	$(\bar{a},\bar{b})=(\bar{z},\bar{z})$
z = ab	$\dot{z}=\dot{a}b+a\dot{b}$	$(ar{a},ar{b})=(ar{z}b,aar{z})$
$(z_1, z_2) = (a, a)$	$(\dot{z}_1,\dot{z}_2)=(\dot{a},\dot{a})$	$\bar{a} = \bar{z}_1 + \bar{z}_2$
Y = AXB	$\dot{Y} = A\dot{Y}B$	$\bar{X} = A^{\mathrm{T}} \bar{Y} B^{\mathrm{T}}$
y = LS(M, m)	$\dot{y} = \mathcal{J} LS(M, m)(y, \dot{M}, \dot{m})$	$(\bar{M}, \bar{m}) = \mathcal{J}^{\mathrm{T}} \operatorname{LS}(M, m)(y, \bar{y})$
	$= LS(M, \dot{m} - \dot{M}y)$	$= (-\bar{m}y^{\mathrm{T}}, \mathrm{LS}(M^{\mathrm{T}}, \bar{y}))$

Table 2: Forward mode AD Transformations.

Type	Primal	Forward Transform
Regular	y = LLS(A, b)	$\dot{y} = \mathcal{J} \operatorname{LLS}(A, b)(y, \dot{A}, \dot{b})$ = $\operatorname{LS}(A^{\mathrm{T}}A, \dot{A}^{\mathrm{T}}b + A^{\mathrm{T}}\dot{b} - (\dot{A}^{\mathrm{T}}A + A^{\mathrm{T}}\dot{A})y)$
"Diff + Sketch"	$y_D = LLS(A, b, S)$	$\dot{y}_D = \mathcal{J} LLS(A, b)(y_D, \dot{A}, \dot{b}, S)$ = $LS(A^T S^T S A, \dot{A}^T b + A^T \dot{b} - (\dot{A}^T A + A^T \dot{A}) y_D)$
"Sketch + Diff"	$y_S = LLS(A, b, S)$	$\dot{y}_S = \mathcal{J} \operatorname{LLS}(A, b)(y_S, \dot{A}, \dot{b}, S)$ $= \operatorname{LS}(A^{\mathrm{T}} S^{\mathrm{T}} S A, \dot{A}^{\mathrm{T}} S^{\mathrm{T}} S b + A^{\mathrm{T}} S^{\mathrm{T}} S \dot{b}$ $- (\dot{A}^{\mathrm{T}} S^{\mathrm{T}} S A + A^{\mathrm{T}} S^{\mathrm{T}} S \dot{A}) y_S)$

Table 3: Reverse mode AD Transformations.

Type	Primal	Reverse Transform
Regular	y = LLS(A, b)	$(\bar{A}, \bar{b}) = \mathcal{J}^{\mathrm{T}} \operatorname{LLS}(A, b)(y, \bar{y})$
		$= (-A^{\dagger \mathrm{T}} \bar{y} y^{\mathrm{T}} - A y \bar{y}^{\mathrm{T}} M^{-1} + b \bar{y}^{\mathrm{T}} M^{-1}, A^{\dagger T} \bar{y})$
"Diff + Sketch"	$y_D = LLS(A, b, S)$	$(\bar{A}, \bar{b}) = \mathcal{J}^{\mathrm{T}} \operatorname{LLS}(A, b)(y, \bar{y})$
		$= (-AM_S^{-1}\bar{y}y_D^{\mathrm{T}} - Ay_D\bar{y}^{\mathrm{T}}M_S^{-1} + b\bar{y}^{\mathrm{T}}M_S^{-1}, A^{\dagger T}\bar{y})$
"Sketch + Diff"	$y_S = LLS_S(A, b, S)$	$(\bar{A}_S, \bar{b}_S) = \mathcal{J}^{\mathrm{T}} \operatorname{LLS}_S(A, b, S)(y_S, \bar{y})$
		$= (-S^{T} A_S^{\dagger T} \bar{y} y_S^{T} - S^{T} S A y_S \bar{y}^{T} M_S^{-1} + S^{T} S b \bar{y}^{T} M_S^{-1}, S^{T} A_S^{\dagger T} \bar{y})$

A.3 "Sketch and Differentiate"

Lemma 2. The reverse mode approximation error for the term \bar{b} when we approximate it by sketching matrix S can be bounded with probability $1 - \delta$ as follows: $\|\bar{b} - \bar{b}_S\|_2 \le \|\Sigma^{-1}\|_2 \|\bar{y}\|_2 (\epsilon + (1 + \epsilon)\|I - S^T S\|_2)$.

Proof. Let us use Lemma 1 and sub-multiplicativity to obtain the following:

$$\|\bar{b} - \bar{b}_{S}\|_{2} = \|AM^{-T}\bar{y} - S^{T}SAM_{S}^{-T}\bar{y}_{S}\|_{2}$$

$$= \|AM^{-1}\bar{y} - AM_{S}^{-1}\bar{y} + AM_{S}^{-1}\bar{y} - S^{T}SAM_{S}^{-1}\bar{y}\|_{2}$$

$$\leq \|AM^{-1} - AM_{S}^{-1}\|_{2}\|\bar{y}\|_{2} + \|I - S^{T}S\|_{2}\|AM_{S}^{-1}\|_{2}\|\bar{y}\|_{2}$$

$$\leq \epsilon \|\Sigma^{-1}\|_{2}\|\bar{y}\|_{2} + \|I - S^{T}S\|_{2}\|AM_{S}^{-1}\|_{2}\|\bar{y}\|_{2}$$

$$\leq \|\Sigma^{-1}\|_{2}\|\bar{y}\|_{2}(\epsilon + (1 + \epsilon)\|I - S^{T}S\|_{2})$$
(11)

where we used a lemma from the main paper. So, the error can be large ($||I - S^T S||_2$).

Lemma 3. The reverse mode approximation error for the term \bar{A} when we approximate it using the sketching matrix S can be bounded with probability $1 - \delta$.

Proof.

$$\|\bar{A} - \bar{A}_S\|_F = \|-2AM^{-T}\bar{y}y^{T} + b\bar{y}^{T}M^{-1} - (-2S^{T}SAM_S^{-T}\bar{y}_Sy_S^{T} + S^{T}Sb\bar{y}_S^{T}M_S^{-1})\|_F$$

$$\leq \|2AM^{-1}\bar{y}y^{T} - 2S^{T}SAM_S^{-1}\bar{y}y_S^{T}\|_F + \|b\bar{y}^{T}M^{-1} - S^{T}Sb\bar{y}^{T}M_S^{-1})\|_F \qquad (12)$$

$$\|AM^{-1}\bar{y}y^{T} - S^{T}SAM_S^{-1}\bar{y}y_S^{T}\|_F \leq \|AM^{-1}\bar{y}y^{T} - AM_S^{-1}\bar{y}y^{T}\|_F + \|AM_S^{-1}\bar{y}y^{T} - S^{T}SAM_S^{-1}\bar{y}y_S^{T}\|_F$$

$$\leq \epsilon \|\Sigma^{-1}\|_F \|\bar{y}\| \|y\| + \|AM_S^{-1}\bar{y}y^{T} - S^{T}SAM_S^{-1}\bar{y}y_S^{T}\|_F \qquad (13)$$

A.4 "Differentiate and Sketch"

Lemma 4. The reverse mode approximation error for the term \bar{b} when we sketch only the computationally expensive terms by S, with probability at least $1 - \delta$, satisfies: $\|\bar{b} - \bar{b}_S\|_2 \lesssim \epsilon \|\Sigma^{-1}\|_2 \|\bar{y}\|_2$.

Proof. Let us use the sketching properties and sub-multiplicativity to obtain the following:

$$\|\bar{b} - \bar{b}_{S}\|_{2} = \|AM^{-T}\bar{y} - AM_{S}^{-T}\bar{y}_{S}\|_{2}$$

$$\approx \|U(I - U^{T}S^{T}SU)\Sigma^{-1}V^{T}\bar{y}\|_{2} \qquad \bar{y} \approx \bar{y}_{S}$$

$$\lesssim \epsilon \|U\|_{2}\|\Sigma^{-1}\|_{2}\|\bar{y}\|_{2}$$

$$\lesssim \epsilon \|\Sigma^{-1}\|_{2}\|\bar{y}\|_{2}$$
(14)

Lemma 5. The reverse mode approximation error for the term \bar{A} when we sketch only the computationally expensive terms by S, with probability 1-1/poly(d), satisfies: $\|\bar{A}-\bar{A}_S\|_2 \lesssim \epsilon \|\bar{y}\|_2 (\|\Sigma^{-1}\|_2 \|y\|_2 + \frac{1}{1-\epsilon} \|\Sigma^{-1}\|_2 \|Ay - b\|_2 \|A^{\dagger}\|_2)$.

Proof. The approximation error can be split into 3 terms such that $\|\bar{A} - \bar{A}_S\| \le Q_1 + Q_2 + Q_3$ where:

$$Q_{1} = \|b\bar{y}^{\mathrm{T}}M^{-1} - b\bar{y}_{S}^{\mathrm{T}}M_{S'}^{-1}\|_{F}$$
$$\leq \epsilon \|b\bar{y}^{\mathrm{T}}\|_{F}\|\Sigma^{-1}\|_{2}\|\Sigma^{-1}\|_{F}$$

Let us bound Q_2 as follows:

$$Q_{2} = \|AM^{-1}\bar{y}y^{T} - AM_{S'}^{-1}\bar{y}y_{S}^{T}\|_{F} = \|A(M^{-1} - M_{S'}^{-1})\bar{y}y^{T} + AM_{S'}^{-1}\bar{y}y^{T} - AM_{S'}^{-1}\bar{y}y_{S}^{T}\|_{F}$$

$$\leq \|A(M^{-1} - M_{S'}^{-1})\bar{y}y^{T}\|_{F} + \|AM_{S'}^{-1}\bar{y}(y - y_{S})^{T}\|_{F}$$

$$\leq \epsilon \|\Sigma^{-1}\|_{2}\|\bar{y}y^{T}\|_{F} + \|AM_{S'}^{-1}\|_{2}\|\bar{y}(y - y_{S})^{T}\|_{F}$$

$$\leq \epsilon \|\Sigma^{-1}\|_{2}\|\bar{y}\|_{2}\|y\|_{2} + \|AM_{S'}^{-1}\|_{2}\|\bar{y}\|_{2}\|(y - y_{S})\|_{2}$$

$$\leq \epsilon \|\bar{y}\|_{2}(\|\Sigma^{-1}\|_{2}\|y\|_{2} + \|AM_{S'}^{-1}\|_{2}\|Ay - b\|_{2}\|A^{\dagger}\|_{2})$$

$$\leq \epsilon \|\bar{y}\|_{2}(\|\Sigma^{-1}\|_{2}\|y\|_{2} + (1 + \epsilon)\|\Sigma^{-1}\|_{2}\|Ay - b\|_{2}\|A^{\dagger}\|_{2})$$

$$(15)$$

where we used the following result Price et al. (2017):

$$||y - y_S||_2 \le \epsilon ||Ay - b||_2 ||A^{\dagger}||_2 \tag{16}$$

and the last term Q_3 can be bounded as:

and the last term
$$Q_3$$
 can be bounded as:
$$Q_3 = \|Ay\bar{y}^{\mathrm{T}}M^{-1} - Ay_S\bar{y}^{\mathrm{T}}M_S^{-1}\| = \|Ay\bar{y}^{\mathrm{T}}(M^{-1} - M_S^{-1}) + Ay\bar{y}^{\mathrm{T}}M_S^{-1} - Ay_S\bar{y}^{\mathrm{T}}M_S^{-1}\|$$

$$\leq \epsilon \|Ay\bar{y}^{\mathrm{T}}\| + \|A(y - y_S)\bar{y}^{\mathrm{T}}M_S^{-1}\|$$

$$\leq \epsilon \|Ay\bar{y}^{\mathrm{T}}\| + \epsilon \|A\| \|Ay - b\| \|\bar{y}^{\mathrm{T}}M_S^{-1}\|$$
(18)

Note that all three terms Q_1, Q_2, Q_3 are $O(\epsilon)$.

B **Experiments**

We plot the performance of the two proposed approaches for obtaining forward and reverse mode AD in the case of linear regression. We generate a linear regression problem by choosing the entries of matrix A and vector b from i.i.d. N(0,1) (Normal distribution with mean 0 and variance 1). The differences from the two approaches, "sketch+differentiate" and "differentiate+sketch" are shown in Figure 1.

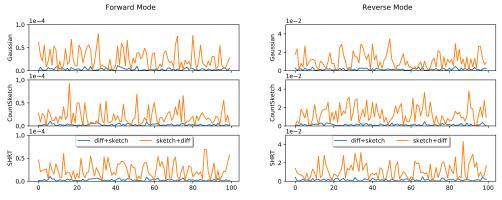


Figure 1: Numerical observation that differentiation and sketching do not commute, and that differentiation-then-sketch is more accurate. We show the forward mode along with its approximation corresponding to the three sketching matrices of Gaussian, Count-sketch and Subsampled Randomized Hadamard Transform (SRHT), on a randomly generated least squares problem of size 100000×100 , along with a random perturbation. Reverse mode is shown for a subsample of 100 randomly chosen values for the variable b, where we used sign as the cost function.

References

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