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Supplement to
SUMMATION BY PARTS, PROJECTIONS, AND STABILITY. I

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Let $P = I - \Sigma^{-1}L(L^T\Sigma^{-1}L)^{-1}L^T$ where $L = \begin{pmatrix} L_{11} & \dots & L_{1r} & L_{0\chi} & L_{21} & \dots & L_{2r} \end{pmatrix}$ represents homogeneous Neumann conditions (localized to the origin), cf. section on the heat equation. For convenience we have $\chi = 0.5$ and $h_1 = h_2 = 1$. We shall show that $L_{10}^T P = 0$, which will follow if we can prove that $L_{10}^T\Sigma^{-1}L(L^T\Sigma^{-1}L)^{-1}L^T = L_{10}^T$. Straightforward computations show that

$$L^T\Sigma^{-1}L = \begin{pmatrix} D_{11} & D_{12} & D_{13} \\ D_{12}^T & D_{22} & D_{23} \\ D_{13}^T & D_{23}^T & D_{33} \end{pmatrix},$$

where

$$D_{11} = D_{33} = \kappa \begin{pmatrix} \frac{1}{\sigma_1} & & \\ & \ddots & \\ & & \frac{1}{\sigma_r} \end{pmatrix}, \quad D_{12} = D_{23}^T = \tau^{-1} \begin{pmatrix} \frac{d_{01}}{\sigma_1} \\ \vdots \\ \frac{d_{0r}}{\sigma_r} \end{pmatrix},$$

and

$$D_{13} = \tau^2 D_{12} D_{23}, \quad D_{22} = \frac{1}{2}\left(\frac{\kappa}{\sigma_0} + \frac{d_{00}^2}{\sigma_0^2}\right), \quad \kappa = \sum_{k=0}^{r} \frac{d_{0k}^2}{\sigma_k}, \quad \tau = \frac{2\sigma_0}{d_{00}}.$$

The inverse is given by

$$(L^T\Sigma^{-1}L)^{-1} = \begin{pmatrix} T_{11} & T_{12} & T_{13} \\ T_{12}^T & T_{22} & T_{23} \\ T_{13}^T & T_{23}^T & T_{33} \end{pmatrix}$$

with

$$T_{11} = T_{33} = D_{11}^{-1} + \frac{\mu}{1-\mu\sigma} D_{11}^{-1} D_{12} D_{12}^T D_{11}^{-1},$$

$$T_{12} = T_{23}^T = \frac{-(\mu - \sigma\tau^4)}{(1-\mu\sigma)(1-\sigma\tau^2)} D_{11}^{-1} D_{12},$$

$$T_{13} = T_{13}^T = \frac{\mu - \tau^2}{(1-\mu\sigma)(1-\sigma\tau^2)} D_{11}^{-1} D_{12} D_{23} D_{33}^{-1},$$

$$T_{22} = \frac{(\mu - \sigma\tau^4)(1+\sigma\tau^2)}{(1-\mu\sigma)(1-\sigma\tau^2)},$$

and

$$\sigma = D_{12}^T D_{11}^{-1} D_{12},$$
$$\mu = \sigma\tau^4 + \frac{1}{\nu}\left(1 - \sigma\tau^2\right)^2,$$
$$\nu = D_{22} - \sigma.$$

Let $\hat{L} = \begin{pmatrix} L_{10} & \dots & L_{1r} & L_{20} & \dots & L_{2r} \end{pmatrix}$. Then

$$L_{10}^T\Sigma^{-1}L(L^T\Sigma^{-1}L)^{-1}L^T = L_{10}^T\Sigma^{-1}\hat{L}\begin{pmatrix} R & S \\ S & R \end{pmatrix}\hat{L}^T,$$

where (using $T_{12}^T = T_{23}$ and $T_{11} = T_{33}$)

$$R = \begin{pmatrix} T_{22}/4 & T_{12}^T/2 \\ T_{12}/2 & T_{11} \end{pmatrix}, \quad S = \begin{pmatrix} T_{22}/4 & T_{12}^T/2 \\ T_{12}/2 & T_{13} \end{pmatrix}.$$

Furthermore,

$$L_{10}^T\Sigma^{-1}\hat{L} = \begin{pmatrix} \kappa/\sigma_0 & 0 & d_{00}^2/\sigma_0^2 & 2D_{12}^T \end{pmatrix}.$$

Using $D_{22} = (\kappa/\sigma_0 + d_{00}^2/\sigma_0^2)/2$, we have

$$L_{10}^T\Sigma^{-1}\hat{L}\begin{pmatrix} R & S \\ S & R \end{pmatrix} =$$

$$\begin{pmatrix} \frac{1}{2}D_{22}T_{22} + D_{12}^TT_{12} & D_{22}T_{12}^T + 2D_{12}^TT_{13} & \frac{1}{2}D_{22}T_{22} + D_{12}^TT_{12} & D_{22}T_{12}^T + 2D_{12}^TT_{11} \end{pmatrix}.$$

But

$$\frac{1}{2}D_{22}T_{22} + D_{12}^TT_{12} = \frac{1}{2}(D_{12}^TT_{12} + D_{22}T_{22} + D_{23}T_{23}^T) = \frac{1}{2},$$

and

$$D_{22}T_{12}^T + 2D_{12}^TT_{13} = 2\left(D_{12}^TT_{13} + D_{22}T_{12}^T + D_{12}^TT_{11}\right) - \left(D_{22}T_{12}^T + 2D_{12}^TT_{11}\right).$$

Observing that $T_{12}^T = T_{23}$, $D_{12}^TT_{11} = D_{23}T_{33}$, we conclude that the first parenthetical expression vanishes. Thus,

$$L_{10}^T\Sigma^{-1}\hat{L}\begin{pmatrix} R & S \\ S & R \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & D_{22}T_{12}^T + 2D_{12}^TT_{13} & \frac{1}{2} & -\left(D_{22}T_{12}^T + 2D_{12}^TT_{13}\right) \end{pmatrix}.$$

Also,

$$D_{22}T_{12}^T + 2D_{12}^TT_{13} = \rho D_{12}^TD_{11}^{-1}, \quad \rho = \frac{2\sigma(\mu - \tau^2) - (\sigma + \nu)(\mu - \sigma\tau^4)}{(1 - \mu\sigma)(1 - \sigma\tau^2)}.$$

Substituting $1 - \sigma\tau^2 = d_{00}^2/(\kappa\sigma_0)$ and the expression for μ yields

$$\rho = -\frac{\kappa\sigma_0}{d_{00}^2},$$

and so

$$\rho D_{12}^TD_{11}^{-1} = -\frac{1}{2d_{00}}\begin{pmatrix} d_{01} & \dots & d_{0r} \end{pmatrix}.$$

Consequently,

$$L_{10}^T\Sigma^{-1}L(L^T\Sigma^{-1}L)^{-1}L^T = \frac{1}{2d_{00}}\begin{pmatrix} d_{00} & -d_{01} & \dots & -d_{0r} & d_{00} & d_{01} & \dots & d_{0r} \end{pmatrix}\hat{L}^T.$$

The jth block column of $\hat{L}^T$ reads

$$c_j^T = \begin{pmatrix} 0 & \dots & 0 & \sum_{k=0}^{r} d_{0k}e_k^T & 0 & \dots & 0 & d_{0j}e_0^T & \dots & d_{0j}e_r^T \end{pmatrix},$$

where the sum is the jth block element of c_j, $j = 0, \dots, r$. Hence,

$$\frac{1}{2d_{00}}\begin{pmatrix} d_{00} & -d_{01} & \dots & -d_{0r} & d_{00} & d_{01} & \dots & d_{0r} \end{pmatrix}c_j = \delta_{j0}\sum_{k=0}^{r} d_{0k}e_k^T,$$

i. e.,

$$L_{10}^T\Sigma^{-1}L(L^T\Sigma^{-1}L)^{-1}L^T = L_{10}^T.$$

In a similar fashion one shows that L_{20} also satisfies the above equation.

The simplest example is obtained by discretizing the Neumann conditions using the standard divided difference D_+ in both coordinate directions, i. e.,

$$\begin{aligned} v_{11} - v_{01} &= 0, \\ v_{11} - v_{10} &= 0, \\ (v_{10} - v_{00})/2 + (v_{01} - v_{00})/2 &= 0, \end{aligned} \tag{1}$$

which leads to

$$\Sigma^{-1}L(L^T\Sigma^{-1}L)^{-1}L^T = \frac{1}{18}\begin{pmatrix} 16 & -4 & 0 & \dots & 0 & -4 & -8 & 0 & \dots & 0 \\ -2 & 14 & 0 & \dots & 0 & -4 & -8 & 0 & \dots & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\ -2 & -4 & 0 & \dots & 0 & 14 & -8 & 0 & \dots & 0 \\ -2 & -4 & 0 & \dots & 0 & -4 & 10 & 0 & \dots & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \end{pmatrix}. \tag{2}$$

Evidently, any vector $v = Pu$, $P = I - \Sigma^{-1}L(L^T\Sigma^{-1}L)^{-1}L^T$, satisfies (1). Furthermore, by (2), $v_{10} - v_{00} = v_{01} - v_{00} = 0$, which also follows directly from (1).

We conclude this Supplement by proving a number of technical lemmas that were used in the paper. Let D be a difference operator satifying a summation-by-parts rule with respect to the scalar product $(u, v)_h = hu^T\Sigma v$, where

$$\Sigma = \begin{pmatrix} \Sigma^{(1)} & & \\ & I & \\ & & \Sigma^{(2)} \end{pmatrix}, \quad \Sigma^{(l)} \in \mathrm{R}^{(r_l+1)d\times(r_l+1)d}, \quad l = 1, 2. \tag{3}$$

Proposition 1.1. *Let D be as above, and define the norm $\|\cdot\|_h = \sqrt{(\cdot,\cdot)_h}$. Then*

$$|v|_\infty^2 \le \epsilon\|Dv\|_h^2 + \left(\epsilon^{-1} + 1 + \mathcal{O}(h)\right)\|v\|_h^2 ,$$

where $\epsilon > 0$.

Proof. Choose k, l such that

$$|v_k|^2 = \min_j(|v_j|^2)\,, \qquad |v_l|^2 = \max_j(|v_j|^2) \equiv |v|_\infty^2\,.$$

Eq. (3) implies that

$$\|v\|_h^2 \ge h\left(\lambda_1|v^{(1)}|^2 + \lambda_2|v^{(2)}|^2\right) + h\sum_{j=r_1+1}^{\nu-r_2}|v_j|^2 ,$$

where $\lambda_{1,2} > 0$ are the smallest eigenvalues of $\Sigma^{(1,2)}$. Note that $\lambda_{1,2}$ are independent of h. Hence,

$$\|v\|_h^2 \ge \left(1 - h\left(r_1(1-\lambda_1) + r_2(1-\lambda_2)\right)\right)|v_k|^2 ,$$

where we have used $h\nu = L = 1$. If $c \equiv r_1(1-\lambda_1) + r_2(1-\lambda_2) \le 0$, one immediately gets $|v_k|^2 \le \|v\|_h^2$. Otherwise, we choose h such that $hc < 1$. Hence,

$$|v_k|^2 \le \frac{1}{1-hc}\|v\|_h^2 \le (1 + Kh)\|v\|_h^2 , \qquad K = \frac{c}{1-h_0c} , \tag{4}$$

for $h \le h_0$, where h_0 is a fixed number such that $h_0c < 1$.

Next, we define a family of norms, which is obtained by shrinking the interior of (3); $\Sigma^{(1,2)}$ remain constant. Allowing a slight abuse of notation, we write these norms as

$$(u,v)_{h,r,s} = h\sum_{j=r}^{s}\sigma_{ij}u_i^Tv_j ,$$

where $r \ge 0$ and $s \le \nu$. Shrinking the interior of D accordingly, one has

$$(v, Dv)_{h,k,l} = |v_l|^2 - |v_k|^2 - (Dv, v)_{h,k,l} ,$$

i. e.,

$$|v|_\infty^2 \le |v_k|^2 + 2\|Dv\|_{h,k,l}\|v\|_{h,k,l} .$$

Obviously, $\|v\|_{h,k,l} \le \|v\|_{h,0,\nu} \equiv \|v\|_h$, whence

$$|v|_\infty^2 \le \epsilon\|Dv\|_h^2 + \left(\epsilon^{-1} + 1 + \mathcal{O}(h)\right)\|v\|_h^2 ,$$

where (4) and the standard algebraic inequality have been used. □

Lemma 1.1. *Let $A = \mathrm{diag}(A_0 \ \ldots \ A_\nu)$, $A_j = A(jh) \in \mathrm{R}^d$. Then*

$$|(u, Av)_h - (A^Tu, v)_h| \le \mathcal{O}(h)\|u\|_h\|v\|_h .$$

Proof. Denote the commutator of Σ and A by $[\Sigma, A]$. Then

$$(u, Av)_h = (A^Tu, v)_h + hu^T[\Sigma, A]v ,$$

where

$$[\Sigma, A] = \begin{pmatrix} [\Sigma^{(1)}, A^{(1)}] & & \\ & 0 & \\ & & [\Sigma^{(2)}, A^{(2)}] \end{pmatrix}$$

with

$$[\Sigma^{(1)}, A^{(1)}] = \begin{pmatrix} 0 & \sigma_{01}(A_1 - A_0) & \ldots & \sigma_{0r}(A_r - A_0) \\ -\sigma_{01}(A_1 - A_0) & 0 & \ldots & \sigma_{1r}(A_r - A_1) \\ \vdots & & & \vdots \\ -\sigma_{0r}(A_r - A_0) & -\sigma_{1r}(A_r - A_1) & \ldots & 0 \end{pmatrix} .$$

The other nonzero block has a similar structure. Assuming that $A(x)$ is differentiable, we can apply the mean value theorem:

$$[\Sigma^{(1)}, A^{(1)}] = h\begin{pmatrix} 0 & \sigma_{01}A'_{10} & \ldots & \sigma_{0r}rA'_{r0} \\ -\sigma_{01}A'_{10} & 0 & \ldots & \sigma_{1r}(r-1)A'_{r1} \\ \vdots & & & \vdots \\ -\sigma_{0r}rA'_{r0} & -\sigma_{1r}(r-1)A'_{r1} & \ldots & 0 \end{pmatrix} .$$

Hence,

$$|(u, Av)_h - (A^Tu, v)_h| \le c|A'|_\infty h^2\left(|u^{(1)}||v^{(1)}| + |u^{(2)}||v^{(2)}|\right) \le \mathcal{O}(h)\|u\|_h\|v\|_h ,$$

which proves the lemma. □

Lemma 1.2. *Let A be as in the previous lemma. Then*

$$|(u, Av)_h| \le |A|_\infty(1 + \mathcal{O}(h))\|u\|_h\|v\|_h ,$$

where $|A|_\infty = \sup|A(x)|$.

Proof. The definition of $(\cdot,\cdot)_h$ implies that $(u, Av)_h = h\tilde{u}^T\tilde{A}\tilde{v}$, where $\tilde{u} = \Sigma^{1/2}u$, $\tilde{v} = \Sigma^{1/2}v$, and $\tilde{A} = \Sigma^{1/2}A\Sigma^{-1/2}$. Taylor expansion yields $\tilde{A} = A + R$,

$$R = \begin{pmatrix} R^{(1)} & & \\ & 0 & \\ & & R^{(2)} \end{pmatrix}$$

with $R^{(l)} = \mathcal{O}(h)$, $l = 1, 2$. Thus,

$$|(u, Av)_h| \le |A|_\infty\|\tilde{u}\|\|\tilde{v}\| + \mathcal{O}(h)\left(\|\tilde{u}^{(1)}\|\|\tilde{v}^{(1)}\| + \|\tilde{u}^{(2)}\|\|\tilde{v}^{(2)}\|\right) ,$$

i. e.,

$$|(u, Av)_h| \leq (|A|_\infty + \mathcal{O}(h))\,\|\tilde{u}\|\,\|\tilde{v}\|,$$

where $\|\cdot\|$ denotes the standard Euclidean norm. Since $\|\tilde{u}\| = \|u\|_h$, $\|\tilde{v}\| = \|v\|_h$, the lemma follows. □

Corollary 1.1. *If, in addition to the hypotheses of Lemma 1.2, one of the following conditions holds:*

(i) Σ *is diagonal* $\mathrm{diag}(\sigma_0 I \ldots \sigma_\nu I)$,

(ii) *The blocks of A satisfy* $A_0 = \ldots = A_{r_1}$ *and* $A_{\nu - r_2} = \ldots = A_\nu$,

then

$$|(u, Av)_h| \leq |A|_\infty \|u\|_h \|v\|_h .$$

Proof. The hypotheses imply that $\hat{A} = A$, and the corollary follows. □

Lemma 1.3. *Let A be as in Lemma 1.1 and assume that one of the following conditions holds:*

(i) Σ *is diagonal* $\mathrm{diag}(\sigma_0 I \ldots \sigma_\nu I)$,

(ii) *The blocks of A satisfy* $A_0 = \ldots = A_{r_1}$ *and* $A_{\nu - r_2} = \ldots = A_\nu$.

If A is symmetric, then

$$(u, [D, A]v)_h \leq \rho([D, A])\|u\|_h \|v\|_h .$$

Proof. According to the definition of the operator norm we have

$$\|[D, A]\|_h^2 = \max_{\|v\|_h = 1} \|[D, A]v\|_h^2 = \max_{\|w\|=1} hw^T C^T C w ,$$

where $w = \Sigma^{1/2} v$, $C = \Sigma^{1/2}[D, A]\Sigma^{-1/2}$. Because of the assumptions on A (or Σ) we have $C = \hat{D}A - A\hat{D}$, where $\hat{D} = \Sigma^{1/2} D \Sigma^{-1/2}$. Summation by parts implies that

$$\Sigma D = D_s + D_a , \quad D_s = \frac{1}{2}\begin{pmatrix} -I & & \\ & 0 & \\ & & I \end{pmatrix}, \quad I \in \mathrm{R}^{d \times d} ,$$

and D_a is an anti-symmetric matrix. Consequently,

$$C = [\Sigma^{-1/2} D_a \Sigma^{-1/2}, A] ,$$

where we have used $[\Sigma^{-1/2} D_s \Sigma^{-1/2}, A] = 0$. Since D_a is anti-symmetric and A symmetric, we have $C^T = C$, i. e.,

$$\|[D, A]\|_h^2 = \max_{\|w\|=1} hw^T C^2 w - \rho(C)^2 .$$

Finally, $C = \Sigma^{1/2}[D, A]\Sigma^{-1/2}$ implies that

$$\|[D, A]\|_h = \rho([D, A]) ,$$

which proves the lemma. □