MATHEMATICAL AIDE MEMOIR FOR DATA ASSIMILATION

DAIMG MSc programme, Univ. of Reading, RNB

1. Vectors and matrices

1.1. Vector representation of information.

$$\mathbf{v} = \begin{pmatrix} v_1 \\ \vdots \\ v_i \\ \vdots \\ v_n \end{pmatrix}, \quad \mathbf{v} \in \mathbb{R}^n, \quad v_i = (\mathbf{v})_i.$$

1.2. Matrix operator.

$$\mathbf{N} = \begin{pmatrix} N_{11} & \cdots & N_{1j} & \cdots & N_{1n} \\ \vdots & \ddots & \vdots & \vdots & \vdots \\ N_{i1} & \cdots & N_{ij} & \cdots & N_{in} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ N_{m1} & \cdots & N_{mj} & \cdots & N_{mn} \end{pmatrix}, \quad \mathbf{N} \in \mathbb{R}^{m \times n}, \quad N_{ij} = (\mathbf{N})_{ij}.$$

$$\mathbf{v}^{\mathrm{b}} = \mathbf{N}\mathbf{v}^{\mathrm{a}}, \quad \mathbf{v}^{\mathrm{b}} \in \mathbb{R}^m, \quad \mathbf{v}^{\mathrm{a}} \in \mathbb{R}^n, \quad v_i^{\mathrm{b}} = \sum_{j=1}^{n} N_{ij} v_j^{\mathrm{a}}, \quad 1 \le i \le m.$$

1.3. Identity/unit matrix.

$$\mathbf{I}_p = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix}, \quad \mathbf{I}_p \in \mathbb{R}^{p \times p}, \quad (\mathbf{I}_p)_{ij} = \delta_{ij}.$$

1.4. Matrix addition.

$$\mathbf{N} = \mathbf{N}^{\mathrm{a}} + \mathbf{N}^{\mathrm{b}}, \quad N_{ij} = N_{ij}^{\mathrm{a}} + N_{ij}^{\mathrm{b}}, \quad \mathbf{N}, \mathbf{N}^{\mathrm{a}}, \mathbf{N}^{\mathrm{b}} \in \mathbb{R}^{m \times n}.$$

1.5. Matrix multiplication.

$$\mathbf{N} = \mathbf{N}^{\mathrm{a}}\mathbf{N}^{\mathrm{b}}, \quad N_{ij} = \sum_{k=1}^{p} N_{ik}^{\mathrm{a}} N_{kj}^{\mathrm{b}}, \quad \mathbf{N} \in \mathbb{R}^{m \times n}, \quad \mathbf{N}^{\mathrm{a}} \in \mathbb{R}^{m \times p}, \quad \mathbf{N}^{\mathrm{b}} \in \mathbb{R}^{p \times n}.$$

In general, matrices are non-commutative $\mathbf{N}^{\mathrm{a}}\mathbf{N}^{\mathrm{b}} \neq \mathbf{N}^{\mathrm{b}}\mathbf{N}^{\mathrm{a}}$. Pre-multiplication by the identity matrix gives $\mathbf{I}_p\mathbf{N}^{\mathrm{b}} = \mathbf{N}^{\mathrm{b}}$ and post-multiplication by the identity matrix gives $\mathbf{N}^{\mathrm{a}}\mathbf{I}_p = \mathbf{N}^{\mathrm{a}}$. Multiplication by a scalar gives $(\alpha\mathbf{N})_{ij} = \alpha N_{ij}$.

1.6. **Matrix adjoint.** The matrix adjoint makes rows into columns (and vice-versa), and does a complex conjugate on each element.

$$\text{If } \mathbf{N}^{\mathrm{b}} = \mathbf{N}^{\mathrm{a}\dagger}, \quad N^{\mathrm{b}}_{ij} = N^{\mathrm{a}*}_{ji}, \quad \mathbf{N}^{\mathrm{b}} \in \mathbb{C}^{m\times n}, \quad \mathbf{N}^{\mathrm{a}} \in \mathbb{C}^{n\times m}.$$

$$\mathbf{N}^{\mathrm{a}} = \begin{pmatrix} N^{\mathrm{a}}_{11} & N^{\mathrm{a}}_{12} & N^{\mathrm{a}}_{13} \\ N^{\mathrm{a}}_{21} & N^{\mathrm{a}}_{22} & N^{\mathrm{a}}_{23} \end{pmatrix}, \quad \mathbf{N}^{\mathrm{b}} = \begin{pmatrix} N^{\mathrm{a}*}_{11} & N^{\mathrm{a}*}_{21} \\ N^{\mathrm{a}*}_{12} & N^{\mathrm{a}*}_{22} \\ N^{\mathrm{a}*}_{13} & N^{\mathrm{a}*}_{23} \end{pmatrix}.$$

If $\mathbf{N}^{\mathrm{a}} = \mathbf{N}^{\mathrm{a}\dagger}$ then matrix $\mathbf{N}^{\mathrm{a}}$ is self-adjoint/Hermitian (only square matrices can be Hermitian). If the matrix is real then the matrix adjoint is the same as the matrix transpose.

1.7. **Matrix transpose.**

$$\text{If } \mathbf{N}^{\mathrm{b}} = \mathbf{N}^{\mathrm{aT}}, \quad N^{\mathrm{b}}_{ij} = N^{\mathrm{a}}_{ji}, \quad \mathbf{N}^{\mathrm{b}} \in \mathbb{R}^{m\times n}, \quad \mathbf{N}^{\mathrm{a}} \in \mathbb{R}^{n\times m}.$$

$$\mathbf{N}^{\mathrm{a}} = \begin{pmatrix} N^{\mathrm{a}}_{11} & N^{\mathrm{a}}_{12} & N^{\mathrm{a}}_{13} \\ N^{\mathrm{a}}_{21} & N^{\mathrm{a}}_{22} & N^{\mathrm{a}}_{23} \end{pmatrix}, \quad \mathbf{N}^{\mathrm{b}} = \begin{pmatrix} N^{\mathrm{a}}_{11} & N^{\mathrm{a}}_{21} \\ N^{\mathrm{a}}_{12} & N^{\mathrm{a}}_{22} \\ N^{\mathrm{a}}_{13} & N^{\mathrm{a}}_{23} \end{pmatrix}.$$

If $\mathbf{N}^{\mathrm{a}} = \mathbf{N}^{\mathrm{aT}}$ then matrix $\mathbf{N}^{\mathrm{a}}$ is symmetric (only square matrices can be symmetric). Symmetric matrices are also Hermitian.

1.8. **Transpose of a product of matrices.**

$$(\mathbf{N}^{\mathrm{a}}\mathbf{N}^{\mathrm{b}})^{\mathrm{T}} = \mathbf{N}^{\mathrm{bT}}\mathbf{N}^{\mathrm{aT}}.$$

1.9. **Matrix inversion.** Let $\mathbf{N}$ be a square $(m = n)$ non-singular matrix.

$$\text{If } \mathbf{v}^{\mathrm{b}} = \mathbf{N}\mathbf{v}^{\mathrm{a}}, \text{ then } \mathbf{v}^{\mathrm{a}} = \mathbf{N}^{-1}\mathbf{v}^{\mathrm{b}}, \quad \mathbf{v}^{\mathrm{a}}, \mathbf{v}^{\mathrm{b}} \in \mathbb{R}^{n}, \quad \mathbf{N} \in \mathbb{R}^{n\times n}.$$

$$\text{In general } (\mathbf{N}^{-1})_{ij} \neq (\mathbf{N})^{-1}_{ij}.$$

For $n = 2$, $\quad \mathbf{N} = \begin{pmatrix} N_{11} & N_{12} \\ N_{21} & N_{22} \end{pmatrix}, \quad \mathbf{N} = \dfrac{1}{\det(\mathbf{N})}\begin{pmatrix} N_{22} & -N_{12} \\ -N_{21} & N_{11} \end{pmatrix}, \quad \det(\mathbf{N}) = N_{11}N_{22} - N_{12}N_{21}.$

If $\mathbf{N}$ is singular then it has a zero determinant and the inverse cannot be found in general.

1.10. **Moore-Penrose generalized inverse.**

$$\mathbf{N}^{+} = \mathbf{N}^{\mathrm{T}}(\mathbf{N}\mathbf{N}^{\mathrm{T}})^{-1}, \quad \mathbf{N} \in \mathbb{R}^{m\times n}, \quad n > m.$$

1.11. **Diagonal matrix.** A matrix is diagonal if $N_{ij} = 0$ if $i \neq j$, $\mathbf{N} \in \mathbb{R}^{m\times n}$. If $\mathbf{N}$ is square $(m = n)$:

$$\mathbf{N} = \mathrm{diag}(\lambda_1, \lambda_2, \ldots) = \begin{pmatrix} \lambda_1 & 0 & \cdots \\ 0 & \lambda_2 & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}.$$

The inverse of a square diagonal matrix is $(\mathbf{N}^{-1})_{ii} = (\mathbf{N})^{-1}_{ii}$, $(\mathbf{N}^{-1})_{ii} = 0$ for $i \neq j$:

$$\begin{pmatrix} N_{11} & 0 & \cdots \\ 0 & N_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}^{-1} = \begin{pmatrix} 1/N_{11} & 0 & \cdots \\ 0 & 1/N_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}.$$

1.12. **Gramian matrix.** A Gramian matrix is symmetric and has the form $\mathbf{N}^{\mathrm{T}}\mathbf{N}$:

$$\mathbf{N}^{\mathrm{T}}\mathbf{N} \in \mathbb{R}^{n\times n}, \quad \mathbf{N} \in \mathbb{R}^{m\times n}, \quad \mathbf{N}^{\mathrm{T}} \in \mathbb{R}^{n\times m}.$$

1.13. **Euclidean vector inner product (scalar product/dot product).**

$$a = \mathbf{v}^{\mathrm{a}} \cdot \mathbf{v}^{\mathrm{b}} = \mathbf{v}^{\mathrm{aT}} \mathbf{v}^{\mathrm{b}} = \left\langle \mathbf{v}^{\mathrm{a}}, \mathbf{v}^{\mathrm{b}} \right\rangle = \sum_{i=1}^{n} v_i^{\mathrm{a}} v_i^{\mathrm{b}}, \quad \mathbf{v}^{\mathrm{a}}, \mathbf{v}^{\mathrm{b}} \in \mathbb{R}^n, \quad a \in \mathbb{R}.$$

$$b = \mathbf{v} \cdot \mathbf{v} = \mathbf{v}^{\mathrm{T}} \mathbf{v} = \langle \mathbf{v}, \mathbf{v} \rangle = \sum_{i=1}^{n} v_i^2 = \|\mathbf{v}\|^2, \quad \mathbf{v} \in \mathbb{R}^n, \quad b \in \mathbb{R}.$$

1.14. **Non-Euclidean vector inner product.**

$$a = \mathbf{v}^{\mathrm{a}} \cdot (\mathbf{C}\mathbf{v}^{\mathrm{b}}) = \mathbf{v}^{\mathrm{aT}} \mathbf{C} \mathbf{v}^{\mathrm{b}} = \left\langle \mathbf{v}^{\mathrm{a}}, \mathbf{v}^{\mathrm{b}} \right\rangle_{\mathbf{C}} = \sum_{i=1}^{n} v_i^{\mathrm{a}} \sum_{j=1}^{m} C_{ij} v_j^{\mathrm{b}}, \quad \mathbf{v}^{\mathrm{a}} \in \mathbb{R}^n, \quad \mathbf{v}^{\mathrm{b}} \in \mathbb{R}^m, \quad \mathbf{C} \in \mathbb{R}^{n \times m}, \quad a \in \mathbb{R}.$$

$$b = \mathbf{v} \cdot (\mathbf{C}\mathbf{v}) = \mathbf{v}^{\mathrm{T}} \mathbf{C} \mathbf{v} = \langle \mathbf{v}, \mathbf{v} \rangle_{\mathbf{C}} = \sum_{i=1}^{n} v_i \sum_{j=1}^{n} C_{ij} v_j = \|\mathbf{v}\|_{\mathbf{C}}^2, \quad \mathbf{v} \in \mathbb{R}^n, \quad \mathbf{C} \in \mathbb{R}^{n \times n}, \quad b \in \mathbb{R}.$$

1.15. **Vector outer product.**

$$\mathbf{N} = \mathbf{v}^{\mathrm{a}} \mathbf{v}^{\mathrm{bT}}, \quad N_{ij} = v_i^{\mathrm{a}} v_j^{\mathrm{b}}, \quad \mathbf{N} \in \mathbb{R}^{m \times n}, \quad \mathbf{v}^{\mathrm{a}} \in \mathbb{R}^m, \quad \mathbf{v}^{\mathrm{b}} \in \mathbb{R}^n.$$

1.16. **Schur/Hadamard product.**

$$\text{For matrices: } \mathbf{N} = \mathbf{N}^{\mathrm{a}} \circ \mathbf{N}^{\mathrm{b}}, \quad N_{ij} = N_{ij}^{\mathrm{a}} N_{ij}^{\mathrm{b}}, \quad \mathbf{N}, \mathbf{N}^{\mathrm{a}}, \mathbf{N}^{\mathrm{b}} \in \mathbb{R}^{m \times n}.$$

$$\text{For vectors: } \mathbf{v} = \mathbf{v}^{\mathrm{a}} \circ \mathbf{v}^{\mathrm{b}}, \quad v_i = v_i^{\mathrm{a}} v_i^{\mathrm{b}}, \quad \mathbf{v}, \mathbf{v}^{\mathrm{a}}, \mathbf{v}^{\mathrm{b}} \in \mathbb{R}^n.$$

1.17. **Orthogonal matrix.** If $\mathbf{V}$ is orthogonal then:

$$\mathbf{V}^{\mathrm{T}} \mathbf{V} = \mathbf{I}_n, \quad \mathbf{V} \in \mathbb{R}^{m \times n}, \quad n \leq m.$$

$$\text{If } n = m \text{ then } \mathbf{V}^{\mathrm{T}} = \mathbf{V}^{-1}.$$

1.18. **The trace of a matrix.** The trace of a square matrix $\mathbf{N}$, $\mathrm{tr}(\mathbf{N})$, is:

$$\mathrm{tr}(\mathbf{N}) = \sum_{i=1}^{n} N_{ii}, \quad \mathbf{N} \in \mathbb{R}^{n \times n}.$$

1.19. **The Sherman-Morrison-Woodbury formula.**

$$\left(\mathbf{A} + \mathbf{C}\mathbf{D}^{\mathrm{T}}\right)^{-1} = \mathbf{A}^{-1} - \mathbf{A}^{-1} \mathbf{C} \left(\mathbf{I} + \mathbf{D}^{\mathrm{T}} \mathbf{A}^{-1} \mathbf{C}\right)^{-1} \mathbf{D}^{\mathrm{T}} \mathbf{A}^{-1}.$$

Replacing $\mathbf{C} \to \mathbf{CB}$ and then setting $\mathbf{C} = \mathbf{D} = \mathbf{H}$ and $\mathbf{A} = \mathbf{R}$, the following useful formula results:

$$\left(\mathbf{B}^{-1} + \mathbf{H}^{\mathrm{T}} \mathbf{R}^{-1} \mathbf{H}\right) \mathbf{B} \mathbf{H}^{\mathrm{T}} = \mathbf{H}^{\mathrm{T}} \mathbf{R}^{-1} \left(\mathbf{R} + \mathbf{H} \mathbf{B} \mathbf{H}^{\mathrm{T}}\right).$$

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2. Functions

2.1. **Scalar valued function of a vector and its derivative.**

$$f(\mathbf{v}), \quad f \in \mathbb{R}, \quad \nabla_{\mathbf{v}} f(\mathbf{v}) = \left(\frac{\partial f}{\partial \mathbf{v}}\right)^{\mathrm{T}} = \begin{pmatrix} \partial f / \partial v_1 \\ \partial f / \partial v_2 \\ \vdots \\ \partial f / \partial v_n \end{pmatrix}, \quad \mathbf{v}, \nabla_{\mathbf{v}} f(\mathbf{v}) \in \mathbb{R}^n.$$

2.2. **Generalised chain rule.**

$$\text{Consider } f(\mathbf{v}^{\mathrm{b}}), \text{ where } \nabla_{\mathbf{v}^{\mathrm{b}}} f(\mathbf{v}^{\mathrm{b}}) \text{ is known}, \quad f \in \mathbb{R}, \quad \mathbf{v}^{\mathrm{b}}, \nabla_{\mathbf{v}^{\mathrm{b}}} f(\mathbf{v}^{\mathrm{b}}) \in \mathbb{R}^m.$$

$$\text{If } \mathbf{v}^{\mathrm{b}} = \mathbf{N}\mathbf{v}^{\mathrm{a}}, \text{ then } \nabla_{\mathbf{v}^{\mathrm{a}}} f(\mathbf{v}^{\mathrm{a}}) = \mathbf{N}^{\mathrm{T}} \nabla_{\mathbf{v}^{\mathrm{b}}} f(\mathbf{v}^{\mathrm{b}}), \quad \mathbf{v}^{\mathrm{a}}, \nabla_{\mathbf{v}^{\mathrm{a}}} f(\mathbf{v}^{\mathrm{a}}) \in \mathbb{R}^n, \quad \mathbf{N} \in \mathbb{R}^{m \times n}.$$

2.3. **Generalised Taylor series for f.** Let $f(\mathbf{v})$ be a linear or non-linear function. The Taylor series of $f(\mathbf{v})$ about $\mathbf{v}$ is:

$$f(\mathbf{v} + \delta\mathbf{v}) = f(\mathbf{v}) + \frac{\partial f}{\partial \mathbf{v}} \delta\mathbf{v} + \frac{1}{2} \delta\mathbf{v}^{\mathrm{T}} \frac{\partial^2 f}{\partial \mathbf{v}^2} \delta\mathbf{v} + \text{higher order terms},$$

$$f \in \mathbb{R}, \quad \mathbf{v}, \frac{\partial f}{\partial \mathbf{v}} \in \mathbb{R}^n, \quad \frac{\partial^2 f}{\partial \mathbf{v}^2} \in \mathbb{R}^{n \times n} \text{ is the Hessian matrix}, \left(\frac{\partial^2 f}{\partial \mathbf{v}^2} \right)_{ij} = \frac{\partial^2 f}{\partial v_i \partial v_j}.$$

2.4. **Vector valued function of a vector.**

$$\mathbf{f}(\mathbf{v}), \quad \mathbf{f} \in \mathbb{R}^m, \quad \mathbf{v} \in \mathbb{R}^n.$$

2.5. **Generalised Taylor series for $\mathbf{f}$.** Let $\mathbf{f}(\mathbf{v})$ be a linear or non-linear function. The Taylor series of $\mathbf{f}(\mathbf{v})$ about $\mathbf{v}$ is:

$$\mathbf{f}(\mathbf{v} + \delta\mathbf{v}) = \mathbf{f}(\mathbf{v}) + \mathbf{F}\delta\mathbf{v} + \text{higher order terms},$$

$$\mathbf{F} = \left.\frac{\partial \mathbf{f}}{\partial \mathbf{v}}\right|_{\mathbf{v}}, \quad F_{ij} = \left.\frac{\partial f_i}{\partial v_j}\right|_{\mathbf{v}}, \quad \mathbf{f} \in \mathbb{R}^m, \quad \mathbf{v} \in \mathbb{R}^n, \quad \mathbf{F} \in \mathbb{R}^{m \times n}.$$

$\mathbf{F}$ is the Jacobian of $\mathbf{f}(\mathbf{v})$ about $\mathbf{v}$ and $\partial f_i / \partial v_j$ are called Fréchet derivatives.

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3. Matrix decompositions

3.1. **Eigenvectors and eigenvalues.** The kth eigenvector ($\mathbf{v}_k$) and eigenvalue (λ_k) of matrix $\mathbf{N}$ satisfies:

$$\mathbf{N}\mathbf{v}_k = \lambda_k, \quad \mathbf{N} \in \mathbb{R}^{n \times n}, \quad \mathbf{v}_k \in \mathbb{R}^n, \quad \lambda_k \in \mathbb{R}, \quad 1 \le k \le n.$$

$$\text{Let } \mathbf{V} = (\mathbf{v}_1, \mathbf{v}_2, \cdots \mathbf{v}_n) = \begin{pmatrix} \\ \mathbf{v}_1 \\ \\ \end{pmatrix} \begin{pmatrix} \\ \mathbf{v}_2 \\ \\ \end{pmatrix} \cdots \begin{pmatrix} \\ \mathbf{v}_n \\ \\ \end{pmatrix}, \quad \Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \cdots \lambda_n),$$

$$\mathbf{N}\mathbf{V} = \mathbf{V}\Lambda, \quad \mathbf{N}, \mathbf{V}, \Lambda \in \mathbb{R}^{n \times n}.$$

If $\mathbf{N}$ is Hermitian (if a real matrix then this is equivalent to $\mathbf{N}$ being symmetric) then $\mathbf{V}$ (the matrix of eigenvectors) is orthogonal (see below), and Λ (the matrix of eigenvalues) is real.

For a general 2×2 matrix:

$$\mathbf{N} = \begin{pmatrix} N_{11} & N_{12} \\ N_{21} & N_{22} \end{pmatrix}, \quad \mathbf{V} = \begin{pmatrix} \alpha_1\gamma_1 & \alpha_2\gamma_2 \\ \alpha_1 & \alpha_2 \end{pmatrix}, \quad \Lambda = \begin{pmatrix} \frac{N_{11}+N_{22}-\beta}{2} & 0 \\ 0 & \frac{N_{11}+N_{22}+\beta}{2} \end{pmatrix},$$

$$\beta = \sqrt{N_{11}^2 - 2N_{11}N_{22} + 4N_{12}N_{21} + N_{22}^2},$$

$$\gamma_1 = \frac{N_{11} - N_{22} - \beta}{2N_{21}}, \quad \gamma_2 = \frac{N_{11} - N_{22} + \beta}{2N_{21}}, \quad \alpha_1 = \frac{1}{\sqrt{\gamma_1^2 + 1}}, \quad \alpha_2 = \frac{1}{\sqrt{\gamma_2^2 + 1}}.$$

3.2. **Singular vectors and singular values.**

$$\mathbf{NV} = \mathbf{U}\Lambda, \quad \mathbf{N}^{\mathrm{T}}\mathbf{U} = \mathbf{V}\Lambda, \quad \mathbf{U}^{\mathrm{T}}\mathbf{U} = \mathbf{I}_p, \quad \mathbf{V}^{\mathrm{T}}\mathbf{V} = \mathbf{I}_p.$$

$$\mathbf{N} \in \mathbb{R}^{m\times n}, \quad \mathbf{V} \in \mathbb{R}^{n\times p}, \quad \mathbf{U} \in \mathbb{R}^{m\times p}, \quad \Lambda \in \mathbb{R}^{p\times p}, \quad , p = \text{rank of } \mathbf{N}.$$

$\mathbf{V}$ is the matrix of right singular vectors of $\mathbf{N}$, $\mathbf{U}$ is the matrix of left singular vectors of $\mathbf{N}$, and Λ is the matrix of singular values of $\mathbf{N}$. The following eigenvalue equations exist for $\mathbf{V}$ and $\mathbf{U}$:

$$\mathbf{N}^{\mathrm{T}}\mathbf{NV} = \mathbf{V}\Lambda, \quad \mathbf{NN}^{\mathrm{T}}\mathbf{U} = \mathbf{U}\Lambda.$$

3.3. **The rank of a matrix.** The rank of $\mathbf{N}$ is the number of independent rows or columns of $\mathbf{N}$ (consider, e.g. the ith column of $\mathbf{N}$ as vector $\mathbf{n}_i$). A column (or row) is dependent if it can be written as a linear combination of the other columns (or rows). The rank of a matrix is also the number of non-zero singular values of $\mathbf{N}$. The rank of a square matrix is also the number of non-zero eigenvalues.

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4. Mean, (co)variance, correlation and Gaussian statistics

4.1. **The variance, standard deviation and mean of a scalar.** Consider a population of N scalars, s^l, $1 \leq l \leq N$. The following are for the variance, var(s), standard deviation, σ_s, and mean, $\langle s\rangle$ (common notations are given)[1]:

$$\mathrm{var}(s) = \left\langle (s - \langle s\rangle)^2 \right\rangle = \overline{(s-\bar{s})^2} = \mathcal{E}\left((s - \mathcal{E}(s))^2\right) \approx \frac{1}{\tilde{N}}\sum_{l=1}^{N}(s^l - \langle s\rangle)^2, \quad \sigma_s = \sqrt{\mathrm{var}(s)},$$

$$\langle s\rangle = \bar{s} = \mathcal{E}(s) \approx \frac{1}{N}\sum_{l=1}^{N} s^l.$$

4.2. **The covariance between two scalars.** Consider two populations, each of N scalars, s^l, t^l, $1 \leq l \leq N$. The following is for the covariance, cov(s,t) (common notations are given)[2]:

$$\mathrm{cov}(s,t) = \langle (s - \langle s\rangle)(t - \langle t\rangle)\rangle = \overline{(s-\bar{s})(t-\bar{t})} = \mathcal{E}\left((s - \mathcal{E}(s))(t - \mathcal{E}(t))\right) \approx \frac{1}{\tilde{N}}\sum_{l=1}^{N}(s^l - \langle s\rangle)(t^l - \langle t\rangle).$$

The covariance between two scalars can be negative, zero or positive.

4.3. **The correlation between two scalars.**

$$\mathrm{cor}(s,t) = \frac{\mathrm{cov}(s,t)}{\sigma_s\sigma_t}, \quad -1 \leq \mathrm{cor}(s,t) \leq 1, \quad \mathrm{cor}(s,s) = 1.$$

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[1] Sample variance and sample mean are those (approximate expressions) given in terms of a finite population (a sample). In the expression for the sample variance, $\tilde{N} = N$ if $\langle s\rangle$ is the exact mean, but $\tilde{N} = N - 1$ if $\langle s\rangle$ is the sample mean.

[2] Sample covariance and sample mean are those (approximate expressions) given in terms of a finite population (a sample). In the expression for the sample covariance, $\tilde{N} = N$ if $\langle s\rangle$ and $\langle t\rangle$ is the exact means, but $\tilde{N} = N - 1$ if $\langle s\rangle$ and $\langle t\rangle$ are the sample means.

4.4. **The covariance matrix between two vectors.** Consider two populations, each of N scalars, $\mathbf{u}^l$, $\mathbf{v}^l$, $1 \leq l \leq N$. The following is for the covariance matrix, $\mathrm{cov}(\mathbf{u}, \mathbf{v})$ (common notations are given):

$$\begin{aligned} \mathrm{cov}(\mathbf{u}, \mathbf{v}) &= \left\langle (\mathbf{u} - \langle \mathbf{u} \rangle)(\mathbf{v} - \langle \mathbf{v} \rangle)^{\mathrm{T}} \right\rangle = \overline{(\mathbf{u} - \bar{\mathbf{u}})(\mathbf{v} - \bar{\mathbf{v}})} = \mathcal{E}\left((\mathbf{u} - \mathcal{E}(\mathbf{u}))(\mathbf{v} - \mathcal{E}(\mathbf{v})) \right), \\ &\approx \frac{1}{N-1} \sum_{l=1}^{N} \left(\mathbf{u}^l - \langle \mathbf{u} \rangle \right) \left(\mathbf{v}^l - \langle \mathbf{v} \rangle \right)^{\mathrm{T}}, \\ (\mathrm{cov}(\mathbf{u}, \mathbf{v}))_{ij} &\approx \frac{1}{N-1} \sum_{l=1}^{N} \left(u_i^l - \langle u_i \rangle \right) \left(v_j^l - \langle v_j \rangle \right), \\ & \mathbf{u} \in \mathbb{R}^m, \quad \mathbf{v} \in \mathbb{R}^n, \quad \mathrm{cov}(\mathbf{u}, \mathbf{v}) \in \mathbb{R}^{m \times n}. \end{aligned}$$

If $\mathbf{u} = \mathbf{v}$, then $\mathrm{cov}(\mathbf{v}, \mathbf{v})$ is the auto-covariance matrix of $\mathbf{v}$, where $\mathbf{v} \in \mathbb{R}^n$, $\mathrm{cov}(\mathbf{v}, \mathbf{v}) \in \mathbb{R}^{n \times n}$. Diagonal elements are variances of each element of $\mathbf{v}$, i.e. $(\mathrm{cov}(\mathbf{v}, \mathbf{v}))_{ii} = \mathrm{var}(v_i)$.

4.5. **The correlation matrix between two vectors.**

$$\mathrm{cor}(\mathbf{u}, \mathbf{v}) = \Sigma_{\mathbf{u}}^{-1} \mathrm{cov}(\mathbf{u}, \mathbf{v}) \Sigma_{\mathbf{v}}^{-1}, \quad \Sigma_{\mathbf{u}} = \mathrm{diag}(\sigma_{u_1}, \sigma_{u_2}, \cdots \sigma_{u_m}), \quad \Sigma_{\mathbf{v}} = \mathrm{diag}(\sigma_{v_1}, \sigma_{v_2}, \cdots \sigma_{v_n}),$$

$$(\mathrm{cor}(\mathbf{u}, \mathbf{v}))_{ij} = \frac{(\mathrm{cov}(\mathbf{u}, \mathbf{v}))_{ij}}{\sigma_{u_i} \sigma_{v_j}}, \quad \mathbf{u} \in \mathbb{R}^m, \quad \mathbf{v} \in \mathbb{R}^n, \quad \mathrm{cor}(\mathbf{u}, \mathbf{v}), \mathrm{cov}(\mathbf{u}, \mathbf{v}) \in \mathbb{R}^{m \times n}.$$

4.6. **Gaussian/normal probability density function.**

$$p(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^n \det(\mathbf{P})}} \exp\left[-\frac{1}{2} \left(\mathbf{x} - \langle \mathbf{x} \rangle \right)^{\mathrm{T}} \mathbf{P}^{-1} \left(\mathbf{x} - \langle \mathbf{x} \rangle \right) \right], \quad \mathbf{P} = \mathrm{cov}(\mathbf{x}, \mathbf{x}).$$

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5. Fourier analysis

5.1. **The Fourier transform.** The real-to-spectral space transform in 1-D (1-D Fourier transform):

$$\bar{f}(k) = \frac{1}{\sqrt{2\pi}} \int f(x) \exp(-ikx) dx, \quad i = \sqrt{-1}.$$

The spectral-to-real transform in 1-D (1-D inverse Fourier transform):

$$f(x) = \frac{1}{\sqrt{2\pi}} \int \bar{f}(k) \exp(ikx) dk.$$

The real-to-spectral space transform in d dimensions:

$$\bar{f}(\mathbf{k}) = \frac{1}{(2\pi)^{d/2}} \int\int\int f(\mathbf{x}) \exp(-i\mathbf{k} \cdot \mathbf{x}) d\mathbf{x}.$$

The spectral-to-real transform in d dimensions:

$$f(\mathbf{x}) = \frac{1}{(2\pi)^{d/2}} \int\int\int \bar{f}(\mathbf{k}) \exp(i\mathbf{k} \cdot \mathbf{x}) d\mathbf{k}.$$

The Fourier transforms rely on the orthogonality relationships:

$$\begin{aligned} \int\int\int \exp(i\mathbf{k} \cdot \mathbf{x}) \exp(-i\mathbf{k}' \cdot \mathbf{x}) d\mathbf{x} &= (2\pi)^d \delta(\mathbf{k} - \mathbf{k}'), \\ \int\int\int \exp(i\mathbf{k} \cdot \mathbf{x}) \exp(-i\mathbf{k} \cdot \mathbf{x}') d\mathbf{k} &= (2\pi)^d \delta(\mathbf{x} - \mathbf{x}'), \end{aligned}$$

and satisfies the convolution theorem:

$$\int g(x-x')f(x')dx' \quad \text{has Fourier transform} \quad 2\pi\bar{g}(k)\bar{f}(k).$$

5.2. **Fourier series.** Fourier series are the discrete versions of the Fourier transforms (real and spectral spaces comprising N discrete points). In 1-D:

$$\bar{f}(k_i) = \frac{1}{\sqrt{N}}\sum_{j=1}^{N} f(x_j)\exp(-ik_ix_j), \quad f(x_j) = \frac{1}{\sqrt{N}}\sum_{i=0}^{N-1}\bar{f}(k_i)\exp(ik_ix_j),$$

$$\sum_{j=1}^{N}\exp(ik_ix_j)\exp(ik_{i'}x_j) = N\delta_{ii'}, \quad \sum_{i=0}^{N-1}\exp(ik_ix_j)\exp(ik_ix_{j'}) = N\delta_{jj'}.$$

Representing $f(x_j)$ as the vector $\mathbf{f}$ and $\bar{f}(k_i)$ as the vector $\bar{\mathbf{f}}$ allows the discrete Fourier series, its inverse, and the orthogonality relations to be written compactly via an orthogonal matrix transform:

$$\bar{\mathbf{f}} = \mathbf{F}\mathbf{f}, \quad \mathbf{f} = \mathbf{F}^{\dagger}\bar{\mathbf{f}}, \quad \mathbf{F}^{\dagger}\mathbf{F} = \mathbf{I}_N, \quad \mathbf{F}\mathbf{F}^{\dagger} = \mathbf{I}_N, \quad \text{where matrix elements } F_{ij} = \frac{1}{\sqrt{N}}\exp(-ik_ix_j).$$

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6. Variational calculus

6.1. **Lagrange multipliers.** Problem: find the stationary point of $f(x_1, x_2, \cdots x_N)$ subject to the constraint $g_m(x_1, x_2, \cdots x_N)$, $1 \leq m \leq M$. This problem has N degrees of freedom and M constraints. The constrained variational problem can be written as (f and g_m are implied functions of $x_1, x_2, \ldots x_N$):

$$\frac{\partial}{\partial x_n}\left(f + \sum_{m=1}^{M} g_m\lambda_m\right) = 0, \quad 1 \leq n \leq N,$$

where λ_m is the Lagrange multiplier associated with the mth constraint. This can be written in the following matrix form:

$$\nabla_{\mathbf{x}}f + \mathbf{G}^{\mathrm{T}}\lambda = 0, \quad \mathbf{x} \in \mathbb{R}^N, \quad \lambda \in \mathbb{R}^M, \quad \mathbf{G} \in \mathbb{R}^{M\times N},$$

where $\mathbf{x} = (x_1, x_2, \ldots x_N)^{\mathrm{T}}$ and $G_{mn} = \partial g_m/\partial x_n$.