Mathematical Tools Refresher Course

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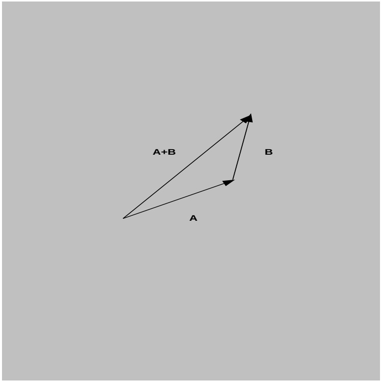
M2 MOCIS/WAPE

Vectors: definitions and superposition principle

Vector $\boldsymbol{A}$ is a coordinate-independent (invariant) object having a magnitude $|\boldsymbol{A}|$ and a direction. Alternative notation $\vec{A}$. Adding/subtracting vectors:



Superposition principle: Linear combination of vectors is a vector.

Products of vectors

Scalar product of two vectors:

Projection of one vector onto another:

$$\boldsymbol{A} \cdot \boldsymbol{B} := |\boldsymbol{A}|\,|\boldsymbol{B}| \cos \phi_{AB} \equiv \boldsymbol{B} \cdot \boldsymbol{A},$$

where ϕ_{AB} is an included angle between the two.

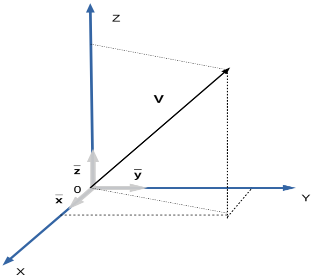
Vector product of two vectors:

$$\boldsymbol{A} \wedge \boldsymbol{B} := \hat{\boldsymbol{i}}_{AB}\,|\boldsymbol{A}|\,|\boldsymbol{B}| \sin \phi_{AB} = -\boldsymbol{B} \wedge \boldsymbol{A},$$

where $\hat{\boldsymbol{i}}_{AB}$ is a unit vector, $|\hat{\boldsymbol{i}}_{AB}| = 1$, perpendicular to both $\boldsymbol{A}$ and $\boldsymbol{B}$, with the orientation of a right-handed screw rotated from $\boldsymbol{A}$ toward $\boldsymbol{B}$.
$\times$ is an alternative notation for $\wedge$.

Distributive properties:
$(\boldsymbol{A}+\boldsymbol{B}) \cdot \boldsymbol{C} = \boldsymbol{A} \cdot \boldsymbol{C} + \boldsymbol{B} \cdot \boldsymbol{C}$, $(\boldsymbol{A}+\boldsymbol{B}) \wedge \boldsymbol{C} = \boldsymbol{A} \wedge \boldsymbol{C} + \boldsymbol{B} \wedge \boldsymbol{C}$.

Vectors in Cartesian coordinates



Cartesian coordinates: defined by a right-hand triad of mutually orthogonal unit vectors forming a basis:

$$(\hat{\boldsymbol{x}},\, \hat{\boldsymbol{y}},\, \hat{\boldsymbol{z}}) \equiv (\hat{\boldsymbol{x}}_1,\, \hat{\boldsymbol{x}}_2,\, \hat{\boldsymbol{x}}_3),$$

Tensor notation and Kronecker delta

$(\hat{\boldsymbol{x}}, \hat{\boldsymbol{y}}, \hat{\boldsymbol{z}}) \to \hat{\boldsymbol{x}}_i,\ i = 1, 2, 3$. Ortho-normality of the basis:

$$\hat{\boldsymbol{x}}_i \cdot \hat{\boldsymbol{x}}_j = \delta_{ij},$$

where δ_{ij} is Kronecker delta-symbol, an invariant tensor of second rank (3×3 unit diagonal matrix):

$$\delta_{ij} = \begin{cases} 1, & \text{if } i = j, \\ 0, & \text{if } i \neq j. \end{cases}$$

The components V_i of a vector $\boldsymbol{V}$ are given by its *projections* on the axes $V_i = \boldsymbol{V} \cdot \hat{\boldsymbol{x}}$:

$$\boldsymbol{V} = V_1 \hat{\boldsymbol{x}}_1 + V_2 \hat{\boldsymbol{x}}_2 + V_3 \hat{\boldsymbol{x}}_3 \equiv \sum_{i=1}^{3} V_i \, \hat{\boldsymbol{x}}_i$$

Einstein's convention:
$\sum_{i=1}^{3} A_i B_i \equiv A_i B_i$ (self-repeating index is "dumb").

Vector products by Levi-Civita tensor

Formula for the vector product:

$$\boldsymbol{A} \wedge \boldsymbol{B} = \left\| \begin{matrix} \hat{\boldsymbol{x}} & \hat{\boldsymbol{y}} & \hat{\boldsymbol{z}} \\ A_1 & A_2 & A_3 \\ B_1 & B_2 & B_3 \end{matrix} \right\|$$

Tensor notation (with Einstein's convention):

$$(\boldsymbol{A} \wedge \boldsymbol{B})_i = \epsilon_{ijk} A_j B_k,$$

where

$$\epsilon_{ijk} = \begin{cases} 1, \text{ if } ijk = 123, 231, 312 \\ -1, \text{ if } ijk = 132, 321, 213 \\ 0, \text{ otherwise} \end{cases}$$

Magic identity:

$$\epsilon_{ijk}\epsilon_{klm} = \delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}. \qquad (1)$$

Scalar, vector, and tensor fields

Any point in space is given by its radius-vector $\boldsymbol{x} = x\hat{\boldsymbol{x}} + y\hat{\boldsymbol{y}} + z\hat{\boldsymbol{z}}$.
A field is an object defined at any point of space $(x, y, z) \equiv (x_1, x_2, x_3)$ at any moment of time t, i.e. a function of $\boldsymbol{x}$ and t.
Different types of fields:

- scalar $f(\boldsymbol{x}, t)$,
- vector $\boldsymbol{v}(\boldsymbol{x}, t)$,
- tensor $t_{ij}(\boldsymbol{x}, t)$

The fields are dependent variables, and x, y, z and t - independent variables.
Physical examples: scalar fields - temperature, density, pressure, geopotential, vector fields - velocity, electric and magnetic fields, tensor fields - stresses, gravitational field.

Differential operations on scalar fields

Partial derivatives:

$$\frac{\partial f}{\partial x} := \lim_{\Delta x \to 0} \frac{f(x + \Delta x, y, z) - f(x, y, z)}{\Delta x},$$

and similar for other independent variables. Differential operator nabla:

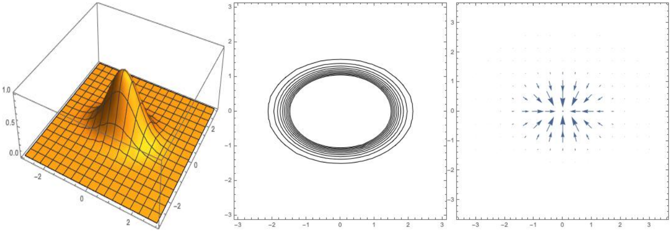
$$\boldsymbol{\nabla} := \hat{\boldsymbol{x}} \frac{\partial}{\partial x} + \hat{\boldsymbol{y}} \frac{\partial}{\partial y} + \hat{\boldsymbol{z}} \frac{\partial}{\partial z}$$

Gradient of a scalar field: the vector field

$$\operatorname{grad} f \equiv \boldsymbol{\nabla} f = \hat{\boldsymbol{x}} \frac{\partial f}{\partial x} + \hat{\boldsymbol{y}} \frac{\partial f}{\partial y} + \hat{\boldsymbol{z}} \frac{\partial f}{\partial z}$$

Heuristic meaning: a vector giving direction and rate of fastest increase of the function f.

Visualizing gradient in 2D



From left to right: 2D relief, its contour map, and its gradient. Graphics by Mathematica©

Differential operations with vectors

- Scalar product: divergence

$$\mathrm{div}\,\boldsymbol{v} \equiv \boldsymbol{\nabla} \cdot \boldsymbol{v}(\boldsymbol{x}) = \frac{\partial v_i}{\partial x_i}$$

- Vector product: curl

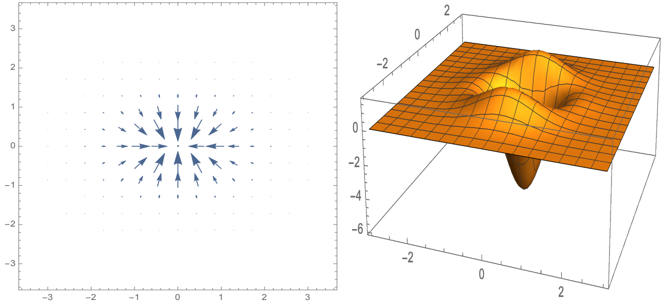
$$\mathrm{curl}\,\boldsymbol{v} \equiv \boldsymbol{\nabla} \wedge \boldsymbol{v}(\boldsymbol{x}); \quad (\mathrm{curl}\,\boldsymbol{v})_i = \epsilon_{ijk} \frac{\partial v_k}{\partial x_j}$$

- Tensor product:

$$\boldsymbol{\nabla} \otimes \boldsymbol{v}(\boldsymbol{x}); \quad (\boldsymbol{\nabla} \otimes \boldsymbol{v})_{ij} = \frac{\partial v_i}{\partial x_j}$$

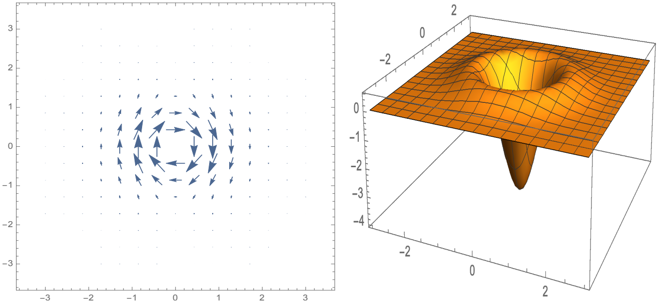
For any $\boldsymbol{v}$, f : $\mathrm{div}\,\mathrm{curl}\,\boldsymbol{v} \equiv 0$, $\mathrm{curl}\,\mathrm{grad}\,f \equiv 0$,
$\mathrm{div}\,\mathrm{grad}\,f = \boldsymbol{\nabla}^2 f$, $\boldsymbol{\nabla}^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ - Laplacian.

Visualizing divergence in 2D



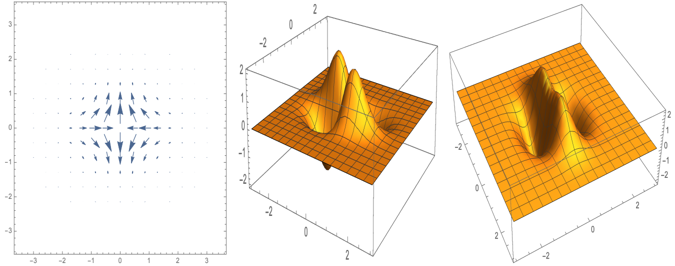
From left to right: vector field $\boldsymbol{v}(x,y) = (v_1(x,y), v_2(x,y))$, and its divergence $\frac{\partial v_1}{\partial x} + \frac{\partial v_2}{\partial y}$. The curl $\hat{\boldsymbol{z}}\left(\frac{\partial v_2}{\partial x} - \frac{\partial v_1}{\partial y}\right)$ of this field is identically zero. (The field is a gradient of the previous example.) Graphics by Mathematica©

Visualizing curl in 2D



From left to right: vector field $\boldsymbol{v}(x, y) = (v_1(x, y), v_2(x, y)),$ and its curl $\frac{\partial v_2}{\partial x} - \frac{\partial v_1}{\partial y}$. The divergence $\frac{\partial v_1}{\partial x} + \frac{\partial v_2}{\partial y}$ of this field is identically zero, so the field is a curl of another vector field. Graphics by Mathematica©

Strain field with non-zero curl and divergence



From left to right: vector field, and its curl and divergence.

Graphics by Mathematica©

Useful identities

$$\nabla \wedge (\nabla \wedge \boldsymbol{v}) = \nabla(\nabla \cdot \boldsymbol{v}) - \nabla^2 \boldsymbol{v}, \qquad (2)$$

$$\boldsymbol{v} \wedge (\nabla \wedge \boldsymbol{v}) = \nabla \left(\frac{\boldsymbol{v}^2}{2} \right) - (\boldsymbol{v} \cdot \nabla)\, \boldsymbol{v}, \qquad (3)$$

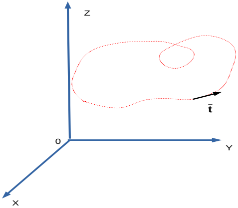
$$\nabla f \cdot (\nabla \wedge \boldsymbol{v}) = -\nabla \cdot (\nabla f \wedge \boldsymbol{v}). \qquad (4)$$

Proofs: using tensor representation $(\nabla \wedge \boldsymbol{v})_i = \epsilon_{ijk}\partial_j v_k$, with shorthand notation $\frac{\partial}{\partial x_i} \equiv \partial_i$, exploiting the antisymmetry of ϵ_{ijk}, using that $\delta_{ij} v_j = v_i$, and applying the magic formula (1).

Example: proof of (2).

$$\epsilon_{ijk}\partial_j \epsilon_{klm}\partial_l v_m = (\delta_{il}\delta_{jm} - \delta_{im}\delta_{jl})\partial_j\partial_l v_m = \partial_i\partial_j v_j - \partial_j\partial_j v_i.$$

Integration of a field along a (closed) 1D contour

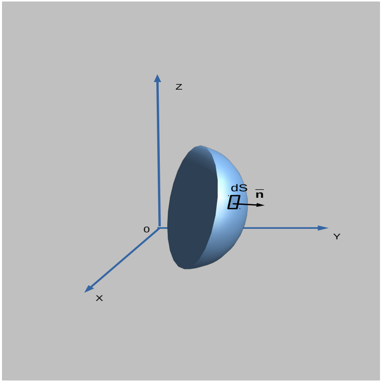


Summation of the values of the field at the points of the contour times oriented line element $d\boldsymbol{l} = \hat{\boldsymbol{t}}\, dl$:

$$\oint d\boldsymbol{l}\,(...),$$

where $\hat{\boldsymbol{t}}$ is unit tangent vector, and dl is a length element along the contour. Positive orientation: anti-clockwise.

Integration of a field over a 2D surface

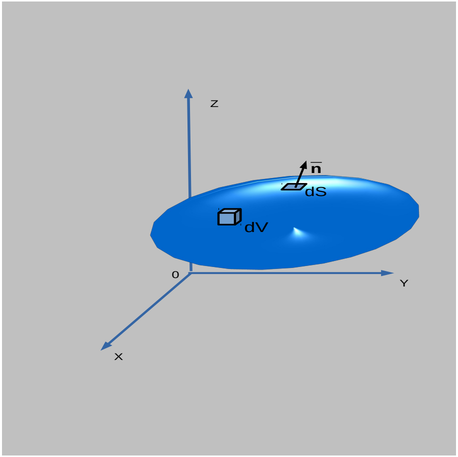


Summation of the values of the field at the points of the surface times oriented surface element $d\boldsymbol{s} = \hat{\boldsymbol{n}}\, ds$:

$$\int\int d\boldsymbol{s}\,(\ldots) \equiv \int_S d\boldsymbol{s}\,(\ldots),$$

where $\hat{\boldsymbol{n}}$ is unit normal vector. Positive orientation for closed surfaces: outwards.

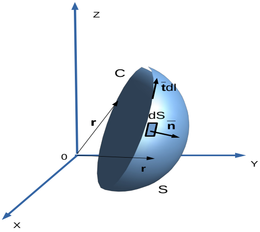
Integration of a field over a 3D volume



Summation of the values of the field at the points in the volume times volume element dV.

$$\int\int\int dV\,(\ldots) \equiv \int_V dV\,(\ldots).$$

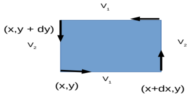
Linking contour and surface integrations: Stokes theorem



$$\oint_C d\boldsymbol{l} \cdot \boldsymbol{v}(\boldsymbol{x}) = \int_{S_C} d\boldsymbol{s} \cdot (\nabla \wedge \boldsymbol{v}(\boldsymbol{x})). \quad (5)$$

Left-hand side: circulation of the vector field over the contour C. Right-hand side: curl of $\boldsymbol{v}$ integrated over any surface S_C having the contour C as a base.

Stokes theorem: the idea of proof



Circulation of the vector $\boldsymbol{v} = v_1 \hat{\boldsymbol{x}} + v_2 \hat{\boldsymbol{y}}$ over an elementary contour, with $dx \to 0$, $dy \to 0$, using first-order Taylor expansions:

$$v_1(x,y)dx + v_2(x+dx,y)dy - v_1(x,y+dy)dx - v_2(x,y)dy = \frac{\partial v_2}{\partial x} dx\, dy - \frac{\partial v_1}{\partial y} dx\, dy,$$

with a z-component of curl$\boldsymbol{v}$ multiplied by the z-oriented surface element arising in the right-hand side.

Linking surface and volume integrations: Gauss theorem

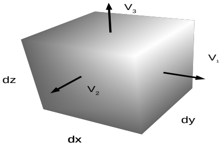
$$\oint_{S_V} d\boldsymbol{s} \cdot \boldsymbol{v}(\boldsymbol{x}) = \int_V dV\, \boldsymbol{\nabla} \cdot \boldsymbol{v}(\boldsymbol{x}). \tag{6}$$

Left-hand side: flux of the vector field through the surface S_V which is a boundary of the volume V. Right-hand side: volume integral of the divergence of the field.

Important. The theorem is also valid for the scalar field:

$$\oint_{S_V} d\boldsymbol{s} \cdot f(\boldsymbol{x}) = \int_V dV\, \boldsymbol{\nabla} f(\boldsymbol{x}). \tag{7}$$

Gauss theorem: the idea of proof



Flux of the vector $\boldsymbol{v} = v_1\hat{\boldsymbol{x}} + v_2\hat{\boldsymbol{y}} + v_3\hat{\boldsymbol{z}}$ over a surface of an elementary volume, taking into account the opposite orientation of the oriented surface elements:

$$[v_1(x+dx,y,z) - v_1(x,y,z)]\,dydz + \\ [v_2(x,y+dy,z) - v_2(x,y,z)]\,dxdz + \\ [v_3(x,y,z+dz) - v_3(x,y,z)]\,dxdy = \left(\frac{\partial v_1}{\partial x} + \frac{\partial v_2}{\partial y} + \frac{\partial v_3}{\partial z}\right) dx\,dy\,dz$$

Curvilinear coordinates

A triple of functions $X^i(x,y,z)$, $i=1,2,3 \Leftrightarrow$ change of variables $(x,y,z) \to (X^1,X^2,X^3) \equiv (X,Y,Z)$. Non zero Jacobian $\mathcal{J}$:

$$\mathcal{J} = \begin{vmatrix} \frac{\partial X}{\partial x} & \frac{\partial X}{\partial y} & \frac{\partial X}{\partial z} \\ \frac{\partial Y}{\partial x} & \frac{\partial Y}{\partial y} & \frac{\partial Y}{\partial z} \\ \frac{\partial Z}{\partial x} & \frac{\partial Z}{\partial y} & \frac{\partial Z}{\partial z} \end{vmatrix} \equiv \frac{\partial(X,Y,Z)}{\partial(x,y,z)} \neq 0.$$

Length element squared (Einstein convention applied):

$$ds^2 = d\boldsymbol{x} \cdot d\boldsymbol{x} \equiv dx^2 + dy^2 + dz^2 = g_{ij}(X_1,X_2,X_3)dX^i dX^j$$

where the metric tensor

$$g_{ij} = \frac{\partial x}{\partial X^i}\frac{\partial x}{\partial X^j} + \frac{\partial y}{\partial X^i}\frac{\partial y}{\partial X^j} + \frac{\partial z}{\partial X^i}\frac{\partial z}{\partial X^j} = g_{ji}.$$

$$g := \det g_{ij} = \left(\frac{\partial(x,y,z)}{\partial(X,Y,Z)}\right)^2 \equiv \mathcal{J}^{-2}.$$

Properties of Jacobians

Volume element:

$$dV = dxdydz = \frac{\partial(x,y,z)}{\partial(X,Y,Z)} dXdYdZ.$$

Consecutive changes of coordinates
$(x, y, z) \to (X, Y, Z) \to (X', Y', Z') \Rightarrow$

$$\frac{\partial(x,y,z)}{\partial(X', Y,' Z')} = \frac{\partial(x,y,z)}{\partial(X,Y,Z)} \cdot \frac{\partial(X,Y,Z)}{\partial(X',Y',Z')}. \qquad (8)$$

Partial changes:

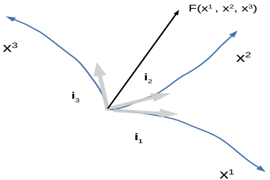
$$\frac{\partial(x,y,z)}{\partial(X,Y,z)} = \frac{\partial(x,y)}{\partial(X,Y)}, \quad \frac{\partial(x,y,z)}{\partial(X,y,z)} = \frac{\partial x}{\partial X}. \qquad (9)$$

Vectors in curvilinear coordinates

Coordinate line: two of X_i fixed, e.g. $i = 2, 3$, curve $(x = x(X^1), y = y(X^1), z = z(X^1))$.

Unit coordinate vectors: unit vectors $\boldsymbol{i}_i$ tangent to respective coordinate lines (*not orthogonal*, in general).

Any vector $\boldsymbol{F} = \hat{F}_1 \boldsymbol{i}_1 + \hat{F}_2 \boldsymbol{i}_2 + \hat{F}_3 \boldsymbol{i}_3$.



Orthogonal coordinates: scalar and vector products

Orthogonality of $\boldsymbol{i}_i \Leftrightarrow g_{ij} = 0, \; i \neq j$
Scalar product of vectors:

$$\boldsymbol{F} \cdot \boldsymbol{G} = \hat{F}_1 \hat{G}_1 + \hat{F}_2 \hat{G}_2 + \hat{F}_3 \hat{G}_3$$

Vector product of vectors:

$$\boldsymbol{F} \wedge \boldsymbol{G} = \begin{vmatrix} \boldsymbol{i}_1 & \boldsymbol{i}_2 & \boldsymbol{i}_3 \\ \hat{F}_1 & \hat{F}_2 & \hat{F}_3 \\ \hat{G}_1 & \hat{G}_2 & \hat{G}_3 \end{vmatrix}.$$

Orthogonal coordinates: differential operations

$$\nabla\Phi = \frac{1}{\sqrt{g_{11}}}\frac{\partial\Phi}{\partial X^1}\boldsymbol{i}_1 + \frac{1}{\sqrt{g_{22}}}\frac{\partial\Phi}{\partial X^2}\boldsymbol{i}_2 + \frac{1}{\sqrt{g_{33}}}\frac{\partial\Phi}{\partial X^3}\boldsymbol{i}_3$$

$$\nabla\cdot\boldsymbol{F} = \frac{1}{\sqrt{g}}\left[\frac{\partial}{\partial X^1}\left(\hat{F}_1\sqrt{\frac{g}{g_{11}}}\right) + \frac{\partial}{\partial X^2}\left(\hat{F}_2\sqrt{\frac{g}{g_{22}}}\right) + \frac{\partial}{\partial X^3}\left(\hat{F}_3\sqrt{\frac{g}{g_{33}}}\right)\right]$$

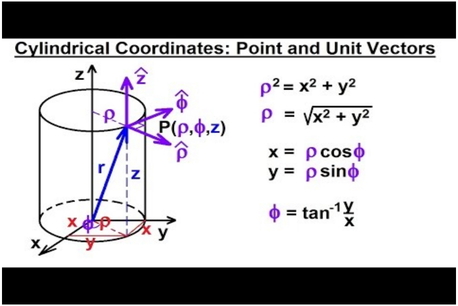
$$\nabla\wedge\boldsymbol{F} = \frac{1}{\sqrt{g}}\begin{vmatrix} \sqrt{g_{11}}\boldsymbol{i}_1 & \sqrt{g_{22}}\boldsymbol{i}_2 & \sqrt{g_{33}}\boldsymbol{i}_3 \\ \frac{\partial}{\partial X^1} & \frac{\partial}{\partial X^2} & \frac{\partial}{\partial X^3} \\ \hat{F}_1\sqrt{g_{11}} & \hat{F}_2\sqrt{g_{22}} & \hat{F}_3\sqrt{g_{33}} \end{vmatrix}.$$

$$\nabla^2\Phi = \frac{1}{\sqrt{g}}\left[\frac{\partial}{\partial X^1}\left(\frac{\sqrt{g}}{g_{11}}\frac{\partial\Phi}{\partial X^1}\right) + \frac{\partial}{\partial X^2}\left(\frac{\sqrt{g}}{g_{22}}\frac{\partial\Phi}{\partial X^2}\right) + \frac{\partial}{\partial X^3}\left(\frac{\sqrt{g}}{g_{33}}\frac{\partial\Phi}{\partial X^3}\right)\right]$$

Important: $\frac{\partial\boldsymbol{i}_j}{\partial X^k} \neq 0$, unlike Cartesian coordinates.

Cylindrical coordinates

$$0 \leq \rho < \infty,\ 0 \leq \phi < 2\pi,\ -\infty < z < +\infty$$



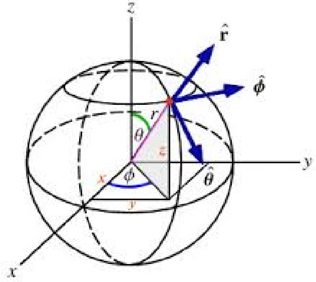
Length element:

$$ds^2 = d\rho^2 + \rho^2 d\phi^2 + dz^2 \ \Rightarrow$$

$$g_{\rho\rho} = 1,\ g_{\phi\phi} = \rho^2,\ g_{zz} = 1 \ \rightarrow \sqrt{g} = \rho.$$

Spherical coordinates

$$0 \leq r < \infty,\ 0 \leq \theta \leq \pi,\ 0 \leq \phi < 2\pi$$



Length element:

$$ds^2 = dr^2 + r^2 d\theta^2 + r^2 \sin^2\theta d\phi^2 \ \Rightarrow$$

$$g_{rr} = 1,\ g_{\theta\theta} = r^2,\ g_{\phi\phi} = r^2\sin^2\theta,\ \rightarrow \sqrt{g} = r^2\sin\theta.$$

Fourier series for periodic functions

Consider $f(x) = f(x + 2\pi)$, a periodic smooth function on the interval $[0, 2\pi]$. Fourier series:

$$f(x) = \sum_{n=0}^{\infty} \left[a_n \cos(n\,x) + b_n \sin(n\,x)\right].$$

The expansion is unique due to ortogonality of the basis functions:

$$\int_0^{2\pi} dx\, \cos(n\,x) \cos(m\,x) = \int_0^{2\pi} dx\, \sin(n\,x) \sin(m\,x) = \pi\delta_{nm},$$

$$\int_0^{2\pi} dx\, \sin(n\,x) \cos(m\,x) \equiv 0.$$

The coefficients of expansion, thus, are uniquely defined:

$$a_n = \frac{1}{\pi} \int_0^{2\pi} dx\, f(x) \cos(n\,x), \quad b_n = \frac{1}{\pi} \int_0^{2\pi} dx\, f(x) \sin(n\,x)$$

Complex exponential form

$$e^{inx} = \cos(n\,x) + i\sin(n\,x) \Rightarrow$$

$$\cos(n\,x) = \frac{e^{inx} + e^{-inx}}{2},\ \sin(n\,x) = \frac{e^{inx} - e^{-inx}}{2i}$$

Hence

$$f(x) = \sum_{n=0}^{\infty} \frac{(a_n - ib_n)}{2} e^{inx} + c.c \equiv \sum_{-\infty}^{\infty} A_n e^{inx},\ A_n^* = A_{-n}$$

Orthogonality:

$$\int_0^{2\pi} dx\, e^{inx} e^{-imx} = 2\pi\delta_{nm}$$

Expression for the complex coefficients

$$A_n = \frac{1}{2\pi}\int_0^{2\pi} dx\, f(x)\, e^{-inx}$$

Fourier integral

Fourier series on arbitrary interval L: $\sin(nx)$, $\cos(nx) \to \sin(\frac{2\pi}{L}nx)$, $\cos(\frac{2\pi}{L}nx)$, $\int_0^{2\pi} dx \to \int_0^L dx$, normalization $\frac{1}{2\pi} \to \frac{1}{L}$. In the limit $L \to \infty$: $\sum_{-\infty}^{\infty} \to \int_{-\infty}^{\infty}$.

Fourier-transformation and its inverse:

$$f(x) = \int_{-\infty}^{\infty} dk\, F(k)\, e^{ikx}, \quad F(k) = \int_{-\infty}^{\infty} dx\, f(x)\, e^{-ikx}.$$

Based on orthogonality:

$$\int_{-\infty}^{\infty} dx\, e^{ikx} e^{-ilx} = \delta(k-l),$$

where $\delta(x)$ - Dirac's delta-function, continuous analog of Kronecker's δ_{nm}, with properties:

$$\int_{-\infty}^{\infty} dx\, \delta(x) = 1, \quad \int_{-\infty}^{\infty} dy\, \delta(x-y)\, F(y) = F(x).$$

Multiple variables and differentiation

$$f(x,y,z) = \int_{-\infty}^{\infty} dk\,dl\,dm\,F(k,l,m)\,e^{i(kx+ly+mz)},$$

$$F(k,l,m) = \int_{-\infty}^{\infty} dx\,dy\,dz\,f(x,y,z)\,e^{-i(kx+ly+mz)}.$$

Physical space $(x,y,z) \longrightarrow (k,l,m)$, Fourier space.
Radius-vector $\boldsymbol{x} \to \boldsymbol{k}$, "wavevector",

$$f(\boldsymbol{x}) = \int_{-\infty}^{\infty} d\boldsymbol{k}\,F(\boldsymbol{k})\,e^{i\boldsymbol{k}\cdot\boldsymbol{x}}$$

Main advantage: differentiation in physical space $\to$ multiplication by the corresponding component of the wave-vector in Fourier space $\frac{\partial}{\partial x} \to ik$:

$$\frac{\partial}{\partial x} f(\boldsymbol{x}) = \int_{-\infty}^{\infty} d\boldsymbol{k}\,ik\,F(\boldsymbol{k})\,e^{i\boldsymbol{k}\cdot\boldsymbol{x}},$$

and similarly for other variables.

Variational derivatives

Variation of a function of $\boldsymbol{x} \in \mathcal{D}$ and $t \in [t_1, t_2]$: $f(\boldsymbol{x}, t) \to f(\boldsymbol{x}, t) + \delta f(\boldsymbol{x}, t)$, $||\delta f(\boldsymbol{x}, t)|| = o(1)$, $||...||$ - a norm (typically L_2). With proper boundary conditions:

$$\delta(\nabla f) = \nabla \delta f, \quad \delta(\partial_t f) = \partial_t \delta f. \tag{10}$$

Variational derivative of a function F of $f(\boldsymbol{x}, t)$: $\frac{\delta F[f(\boldsymbol{x},t)]}{\delta f(\boldsymbol{x}',t')}$.
Important:

$$\frac{\delta f(\boldsymbol{x}, t)}{\delta f(\boldsymbol{x}', t')} = \delta(\boldsymbol{x} - \boldsymbol{x}')\,\delta(t - t') \tag{11}$$

Functionals of $f(\boldsymbol{x}, t)$ and their derivatives:

$$\mathcal{F} = \int_{t_1}^{t_2} dt \int_{\mathcal{D}} d^3\boldsymbol{x} F\left[f(\boldsymbol{x}, t), \nabla f(\boldsymbol{x}, t), \partial_t f(\boldsymbol{x}, t)\right]$$

.

Variations of functionals

Variation of a functional:

$$\delta\mathcal{F} = \int_{t_1}^{t_2} dt' \int_{\mathcal{D}} d^3\boldsymbol{x}' \, \frac{\delta\mathcal{F}}{\delta f(\boldsymbol{x}', t')} \delta f(\boldsymbol{x}', t').$$

Using (11) and integrating by parts in space and time, using vanishing of the variations at the boundaries:

$$\delta\mathcal{F} = \int_{t_1}^{t_2} dt \int_{\mathcal{D}} d^3\boldsymbol{x} \left[\frac{\delta F}{\delta f} - \boldsymbol{\nabla} \cdot \frac{\delta F}{\delta \boldsymbol{\nabla} f} - \partial_t \frac{\delta F}{\delta \partial_t f} \right] \delta f, \quad (12)$$

Invariance of the functional with respect to variations of f $\delta\mathcal{F} = 0 \Rightarrow$ Euler-Lagrange equations:

$$\frac{\delta F(f, \boldsymbol{\nabla} f, \partial_t f)}{\delta f} - \boldsymbol{\nabla} \cdot \frac{\delta F(f, \boldsymbol{\nabla} f, \partial_t f)}{\delta \boldsymbol{\nabla} f} - \partial_t \frac{\delta F(f, \boldsymbol{\nabla} f, \partial_t f)}{\delta \partial_t f} = 0. \quad (13)$$

General first-order ODE

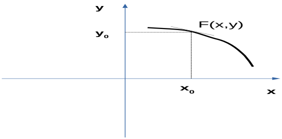
Notation:

$$(\ldots)' \equiv \frac{d\,(\ldots)}{d\,x},\ (\ldots)'' \equiv \frac{d^2\,(\ldots)}{d\,x^2},\ \ldots$$

Typical equation for a function $y(x)$

$$y'(x) = F(x,\ y)$$

Geometric interpretation: field of directions in the x, y plane determined by their slopes $F(x, y)$



Integral curves: $\Phi(x, y, C)$, where C - integration constants determined by b.c. at point x_0: $y(x_0) = y_0$.

Linear first-order ODE

General linear inhomogeneous equation:

$$y'(x) + a(x)y(x) = b(x).$$

Homogeneous equation $\leftrightarrow$ $b(x) \equiv 0$.
General solution:

$$y(x) = \frac{1}{\mu(x)} \left(\int dx\, \mu(x)\, b(x) + C \right)$$

where

$$\mu(x) = e^{\int dx\, a(x)}$$

Linear second-order ODE

General inhomogeneous equation:

$$y''(x) + a(x)y'(x) + b(x)y(x) = c(x). \tag{14}$$

General solution: sum of a particular solution of (14) and of a general solution of the corresponding homogeneous equation

$$y''(x) + a(x)y'(x) + b(x)y(x) = 0. \tag{15}$$

Self-adjoint form of (15):

$$\big(p(x)\, y'(x)\big)' + q(x)y(x) = 0, \tag{16}$$

where

$$p(x) = e^{\int dx\, a(x)},\ q(x) = b(x)\, p(x). \tag{17}$$

General solution of a homogeneous equation and boundary conditions

If one solution of (15) $y_1(x)$ is known, then general solution is:

$$y(x) = y_1(x) \left(C_1 + C_2 \int dx \, \frac{1}{y_1^2(x)\, p(x)} \right), \qquad (18)$$

where $C_{1,2}$ - integration constants.
Can be determined from boundary conditions (b.c.).
Two typical sets of b.c.

- At a given point (initial-value problem): $y(x_0) = A$, $y'(x_0) = B$,
- At the boundary of the interval (boundary-value problem): $y(x_1) = A$, $y(x_2) = B$

General solution of homogeneous equation

Fundamental system of solutions of (15): a pair of linearly independent particular solutions $y_{1,2}(x)$ with

$$W(x) = y_1(x)y_2'(x) - y_2(x)y_1'(x) \neq 0, \qquad (19)$$

where W is Wronskian.
General solution of (14):

$$y(x) = C_1 y_1(x) + C_2 y_2(x) + y_2 \int dx\, \frac{y_1(x)c(x)}{W(x)} - y_1 \int dx\, \frac{y_2(x)c(x)}{W(x)}, \qquad (20)$$

where $C_{1,2}$ - integration constants.

Sturm-Liouville problem

Linear problem on eigenvalues λ and eigenfunctions ϕ_λ:

$$\left(p(x)\,\phi'(x)\right)' + q(x)\phi(x) = \lambda B(x)\phi \qquad (21)$$

on the interval $a < x < b$, with general homogeneous

$$\alpha_1\phi'(a) + \beta_1\phi(a) = 0,\ \alpha_2\phi'(b) + \beta_2\phi(b) = 0, \qquad (22)$$

or periodic b.c.:

$$\phi(a) = \phi(b),\ \phi'(a) = \phi'(b). \qquad (23)$$

Eigenvalues (spectrum) λ_n, $\lambda_1 \le \lambda_2 \le \dots$:

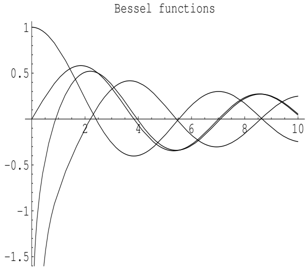
- Real
- $n =$ number of zeros of ϕ_n in $[a, b]$,
- Rank (number of different eigenfunctions per eigenvalue): 1 for (22), 2 for (23)

Eigenfunctions: orthogonal basis of functions in $[a, b]$.

Bessel equation and Bessel functions

$$y''(x) + \frac{1}{x}y'(x) + \left(1 - \frac{m^2}{x^2}\right)y(x) = 0. \qquad (24)$$

Fundamental system of solutions (eigenfunctions with integer eigenvalues $m = 0, 1, 2, ...$ in the interval $0 \leq x < \infty$): Bessel and Neumann functions J_m and N_m:



Hankel functions: $H_m^{1,2}(x) = J_m(x) \pm iN_m(x)$.

Hypergeometric equations and functions

Gauss's equation:

$$x\,(x-1)\,y''(x)+[c-(a+b+1)\,x]\,y'(x)-a\,b\,y(x)=0 \quad (25)$$

Fundamental solution: hypergeometric function given by the hypergeometric series

$$y(x)=F(a,b,c;x)=1+\frac{ab}{c}x+\frac{1}{2!}\,\frac{a(a+1)\,b(b+1)}{c(c+1)}x^2+\dots \quad (26)$$

Second solution - by the receipt given above.

Kummer's equation:

$$x\,y''(x)+(b-x)\,y'(x)-a\,y(x)=0 \quad (27)$$

Fundamental solution: confluent hypergeometric function

$$y(x)=M(a,b;x)=1+\sum_{1}^{\infty}\frac{a^{(n)}}{b^{(n)}\,n!}x,\;\; a^{(n)}=a(a+1)\dots(a+n-1). \quad (28)$$

Second solution $U(a,b;x)$ - by the receipt above.

Example of linear PDE: wave equation

$$u_t + cu_x = 0. \tag{29}$$

$u(x,t)$ in $-\infty < x < +\infty$, and t: $0 \le t < \infty$, $c = \text{const}$.
Notation: $(...)_x = \frac{\partial(...)}{\partial x}$, $(...)_t = \frac{\partial(...)}{\partial t}$
Method of solution 1: change of variables:

$$(x,\, t) \to (\xi_+,\, \xi_-) = (x + ct,\, x - ct)\,. \tag{30}$$

$$\frac{\partial \xi_\pm}{\partial x} = 1, \quad \frac{\partial \xi_\pm}{\partial t} = \pm c \;\Rightarrow \tag{31}$$

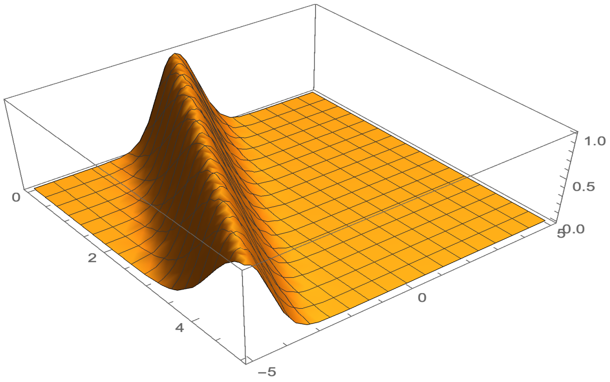
$$\frac{\partial u}{\partial t} = c\left(\frac{\partial u}{\partial \xi_+} - \frac{\partial u}{\partial \xi_-}\right), \quad \frac{\partial u}{\partial x} = \frac{\partial u}{\partial \xi_+} + \frac{\partial u}{\partial \xi_-} \tag{32}$$

$$u_t + cu_x = 0 \to 2c\frac{\partial u}{\partial \xi_+} = 0 \;\Rightarrow u = u(\xi_-). \tag{33}$$

u determined by initial conditions:

$$\text{c.I.} : u_{t=0} = u_0(x) \Rightarrow u = u_0(x - ct). \tag{34}$$

Spatio-temporal evolution of initially localized perturbation



Solution in the domain $-5 < x < 5$, $0 < t < 5$. Initial Gaussian perturbation propagates along a characteristic line with a slope c. Graphics by Mathematica©

Solution by Fourier method

Fourier transformation:

$$u(x,t) = \frac{1}{2\pi} \int dk\, d\omega\, e^{i(kx-\omega t)} \hat{u}(k,\omega) + c.c.. \qquad (35)$$

Inverse:

$$\hat{u}(k,\omega) = \frac{1}{2\pi} \int dx\, dt\, e^{-i(kx-\omega t)} u(x,t) + c.c.. \qquad (36)$$

Fourier-modes: $\hat{u}(k,\omega)e^{i(kx-\omega t)} \leftrightarrow$ - elementary waves.

$$u_t + cu_x = 0 \Rightarrow i\,(kc-\omega)\,\hat{u}(k,\omega),\ \hat{u}(k,\omega) \neq 0 \Rightarrow \qquad (37)$$

General solution:

$$u(x,t) = \frac{1}{2\pi} \int dk\ e^{ik(x-ct)} \hat{u}(k) + c.c. \qquad (38)$$

$\hat{u}(k)$ - Fourier-transform of $u(x,0)$.

Quasi-linear and hyperbolic systems

Quasi-linear system of 1st-order PDE:

$$\partial_t V_i(x,t) + M_{ij}(\boldsymbol{V})\,\partial_x V_j(x,t) = R_i(\boldsymbol{V}),\ \ i,j = 1,2,...,N \tag{39}$$

$\boldsymbol{l}^{(\alpha)}$ - left eigenvectors, $\xi^{(\alpha)}$ - left eigenvalues of M, $\alpha = 1, 2, ...$:

$$\boldsymbol{l}^{(\alpha)} \cdot M = \xi^{(\alpha)} \boldsymbol{l}^{(\alpha)} \ \Rightarrow \tag{40}$$

$$\boldsymbol{l}^{(\alpha)} \cdot \left(\partial_t \boldsymbol{V} + M \cdot \partial_x \boldsymbol{V}\right) = \boldsymbol{l}^{(\alpha)} \cdot \left(\partial_t \boldsymbol{V} + \xi^{(\alpha)} \partial_x \boldsymbol{V}\right). \tag{41}$$

Characteristic directions $\rightarrow$ characteristic curves: $\frac{dx}{dt} = \xi^{(\alpha)}$. Advection along a characteristic:

$$\dot{\boldsymbol{V}} \equiv \frac{d\boldsymbol{V}}{dt} = \left(\partial_t + \xi^{(\alpha)} \partial_x\right) \boldsymbol{V}, \Rightarrow \boldsymbol{l}^{(\alpha)} \cdot \dot{\boldsymbol{V}} = \boldsymbol{l}^{(\alpha)} \cdot \boldsymbol{R}, \tag{42}$$

Les PDE became a system of ODE!

Hyperbolic system: if M has N real and different eigenvalues $\xi^{(\alpha)}$. If $\boldsymbol{l}^{(\alpha)} = \text{const} \rightarrow$ Riemann variables (which become invariants if $\boldsymbol{R} = 0$):

$$r^{(\alpha)} = \boldsymbol{l}^{(\alpha)} \cdot \boldsymbol{V}, \quad \dot{r}^{(\alpha)} = \boldsymbol{l}^{(\alpha)} \cdot \boldsymbol{R}. \tag{43}$$

(Quasi-) linear second-order PDEs

General linear 2nd order equation:

$$a_{11}\frac{\partial^2 f(x,y)}{\partial x^2} + 2a_{12}\frac{\partial^2 f(x,y)}{\partial x \partial y} + a_{22}\frac{\partial^2 f(x,y)}{\partial y^2} = R(x,y) \tag{44}$$

$a_{ij} = a_{ij}(x,y)$. Quasi-linear equation: R and a_{ij} are also functions of f.

- Hyperbolic: $a_{11}a_{22} - a_{12}^2 < 0, \forall(x,y)$
- Parabolic: $a_{11}a_{22} - a_{12}^2 = 0, \forall(x,y)$
- Elliptic: $a_{11}a_{22} - a_{12}^2 > 0, \forall(x,y)$

Second-order 1D wave equation

$$u_{tt} - c^2 u_{xx} = 0. \tag{45}$$

Same change of independent variables as in the 1st-order equation:

$$(x,\, t) \to (\xi_+,\, \xi_-) = (x + ct,\, x - ct)$$

.

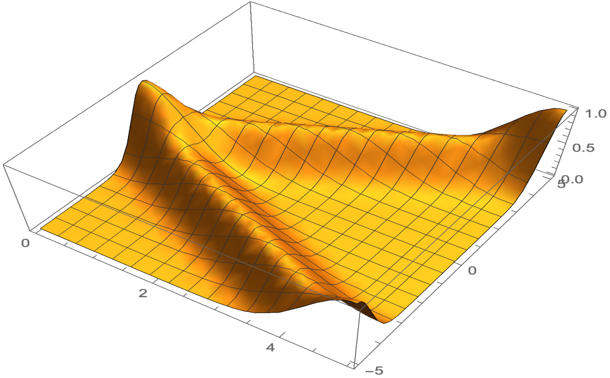
$$u_{tt} - c^2 u_{xx} = 0 \to 4c^2 \frac{\partial^2 u}{\partial \xi_+ \partial \xi_-} = 0 \;\Rightarrow \tag{46}$$

General solution:

$$u = u_-(\xi_-) + u_+(\xi_+), \tag{47}$$

where $u_- + u_+$ - arbitrary functions, to be determined from initial conditions. (2nd order $\Rightarrow$ 2 initial conditions required.)

Spatio-temporal evolution of initially localized perturbation



Solution in the domain $-5 < x < 5$, $0 < t < 5$. Initial Gaussian perturbation propagates along a pair of characteristic lines with slopes $\pm c$. Graphics by Mathematica©

1D heat equation

$$u_t - \kappa^2 u_{xx} = 0,\ \ \kappa = \text{const.} \tag{48}$$

Solution by Fourier method:

$$u(x,t) = \frac{1}{2\pi} \int dk\, e^{ikx} \hat{u}(k,t).\ \rightarrow \tag{49}$$

$$\hat{u}_t(k,t) + \kappa^2 k^2 \hat{u}(k,t) = 0,\ \ \kappa = \text{const.} \rightarrow \tag{50}$$

$$\hat{u}(k,t) = e^{-t\kappa^2 k^2} \hat{u}(k,0), \tag{51}$$

where

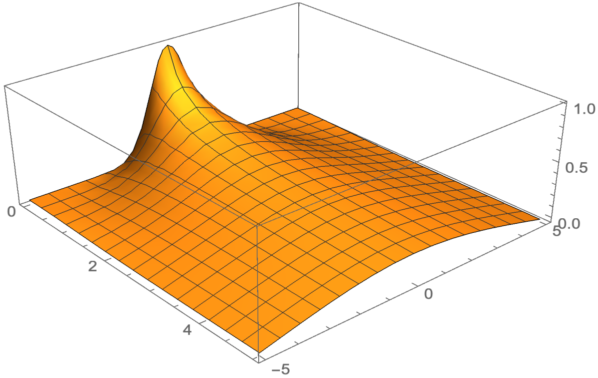
$$\hat{u}(k,0) = \int dx\, e^{-ikx} u_0(x),\ \ u_0(x) \equiv u(x,0) \tag{52}$$

Hence

$$u(x,t) = \frac{1}{2\pi} \int dk\, dx'\, u_0(x')\, e^{ik(x-x')} e^{-t\kappa^2 k^2} \tag{53}$$

$$u(x,t) \propto \frac{1}{\sqrt{t}} \int dx'\, u_0(x')\, e^{-\frac{(x-x')^2}{4\kappa^2 t}} \tag{54}$$

Spatio-temporal evolution of the initial localised perturbation



Solution in the domain $-5 < x < 5$, $0 < t < 5$. Dispersion of initial Gaussian perturbation . Graphics by Mathematica©

2D Laplace equation

$$\nabla^2 f(x,y) = \frac{\partial^2 f(x,y)}{\partial x^2} + \frac{\partial^2 f(x,y)}{\partial y^2} = 0. \qquad (55)$$

In polar coordinates $(r,\,\phi)$:

$$\frac{\partial^2 f(r,\phi)}{\partial r^2} + \frac{1}{r}\frac{\partial f(r,\,\phi)}{\partial r} + \frac{1}{r^2}\frac{\partial^2 f(r,\,\phi)}{\partial \phi^2} = 0. \qquad (56)$$

Separation of variables: $f(r,\phi) = \sum_{m=0}^{\infty} \hat{f}(r) e^{im\phi} + \text{c.c.}, \rightarrow$

$$\hat{f}''(r) + r^{-1}\,\hat{f}'(r) - m^2\, r^{-2}\,\hat{f}(r) = 0,\ (...)' = d(...)/dr. \quad (57)$$

General solution of (57): $\hat{f}(r) = C_1 r^m + C_2 r^{-m}$. At $m \neq 0$ singular at 0 and/or ∞. Solution in a disk $r = r_0$ with b.c. $f(r,\,\phi)|_{r=r_0} = f_0(\phi) = \sum_{m=0}^{\infty} f_m e^{im\phi} + \text{c.c.}$:

$$f(r,\phi) = \sum_{m=0}^{\infty} f_m \left(\frac{r}{r_0}\right)^m e^{im\phi} + \text{c.c.}.$$

Method of Green's functions

General inhomogeneous linear problem:

$$\hat{\mathcal{L}} \circ \mathcal{F} = \mathcal{R} \tag{58}$$

Here $\hat{\mathcal{L}}$ is a linear operator acting on (a set of) function(s) $\mathcal{F}$, the unknowns, $\mathcal{R}$ is a known source/forcing term.
Homogeneous problem: $\mathcal{R} \equiv 0$.
Inverse operator $\hat{\mathcal{L}}^{-1}$ - solution of the problem:

$$\hat{\mathcal{L}}^{-1} \circ \hat{\mathcal{L}} = \mathcal{I}, \tag{59}$$

where $\mathcal{I}$ is unity in functional space. General solution of (58):

$$\mathcal{F} = \hat{\mathcal{L}}^{-1} \circ \mathcal{R} + \mathcal{F}_0, \tag{60}$$

where $\mathcal{F}_0$ - solution of the homogeneous problem.
PDEs context:
Inverse operator = Green's function, $\mathcal{I}$ = delta function.

Poisson equation

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)F(x,y)=R(x,y) \tag{61}$$

Solution in terms of Green's function $\mathcal{G}(x-x', y-y')$:

$$F(x,y)=\int\int dx'dy'\,\mathcal{G}(x-x',y-y')R(x',y'), \tag{62}$$

where

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\mathcal{G}(x-x',y-y')=\delta(x-x')\delta(y-y')\equiv\delta(\boldsymbol{x}-\boldsymbol{x'}) \tag{63}$$

Calculation of $\mathcal{G}$ in the whole $x-y$ plane: put the origin at $\boldsymbol{x'}$, use translational and rotational invariance $\Rightarrow$ $\mathcal{G}=\mathcal{G}(|\boldsymbol{x}|)$, and hence $\boldsymbol{\nabla}\mathcal{G}\parallel\boldsymbol{x}$, use $\boldsymbol{\nabla}^2\ldots\equiv\boldsymbol{\nabla}\cdot(\boldsymbol{\nabla}\ldots)$, integrate both sides of (63) over a circle around the origin, apply Gauss theorem to the left-hand side, and get:

$$\mathcal{G}(\boldsymbol{x})=\frac{1}{2\pi}\log|\boldsymbol{x}|. \tag{64}$$

Green's function for 1D wave equation

$$\left(\frac{\partial^2}{\partial t^2} - c^2\frac{\partial^2}{\partial x^2}\right)\mathcal{G}(x-x', t-t') = \delta(x-x')\delta(t-t') \quad (65)$$

Fourier-transformation

$$\mathcal{G}(x-x', t-t') = \frac{1}{(2\pi)^2}\int\int_{-\infty}^{+\infty} dk d\omega\, \hat{\mathcal{G}}(k,\omega) e^{i(k(x-x')-\omega(t-t'))}$$

Transformed equation:

$$\left(c^2k^2 - \omega^2\right)\hat{\mathcal{G}}(k,\omega) = 1, \Rightarrow \quad (66)$$

$$\mathcal{G}(x-x', t-t') = \frac{1}{(2\pi)^2}\int\int_{-\infty}^{+\infty} dk d\omega\, \frac{e^{i(k(x-x')-\omega(t-t'))}}{c^2k^2-\omega^2}. \quad (67)$$

Integral is singular at $\omega_{\pm} = \pm c\,k$ - how to proceed?

Calculation in the complex ω-plane: general idea

Integral over the real ω- axis $\int_{\mathcal{R}} d\omega\,(...)$ is equal to integral over the contour $\mathcal{C}$ in complex ω plane.

$$\oint_{\mathcal{C}} d\omega\,(...) \equiv \int_{\mathcal{R}} d\omega\,(...) + \int_{\mathcal{A}} d\omega\,(...)$$

where $\mathcal{C} = \mathcal{R} + \mathcal{A}$, $\mathcal{A}$: a semi-circle in the complex plane ending at $\pm\infty$ on $\mathcal{R}$, if $\int_{\mathcal{A}} d\omega\,(...) = 0$, and situated either in upper or in lower half-plane.

Calculation in the complex ω-plane: residue theorem

$f(z)$: function of complex variable z, with a simple pole $f \propto \frac{1}{z-c}$ inside the contour $\mathcal{C}$.

$$\frac{1}{2\pi i} \oint_{\mathcal{C}} dz\, f(z) = \lim|_{z \to c} (z - c) f(z)$$

Denominator in (67): $\frac{1}{c\,k} \left(\frac{1}{\omega - ck} - \frac{1}{\omega + ck} \right)$ - a pair of poles at $\omega = \omega_{\pm} = \pm ck$. In order to apply the theorem, they should be understood as $\omega_{\pm} = \lim|_{\epsilon \to 0} (\omega_{\pm} + i\epsilon)$, where the sign of ϵ is to be determined.

Causality principle

Causality: reaction after the action $\Rightarrow$ Green's function $\neq 0$ only when $t - t' > 0$.

At the semicircle of radius $R \to \infty$:
$\omega = Re^{i\Phi}$, $d\omega = iR\, d\Phi$, where Φ is the polar angle. The denominator of the ω- integral in (67) $\sim R^2$. If numerator is bounded, which depends on the sign of the exponent, and is true for the lower (upper) semicircle if $t - t' > 0$ ($t - t' < 0$), the integral over semicircle $\propto \frac{1}{R}\Big|_{R\to\infty} \to 0$. Correspondingly, if $\epsilon < 0$ integral $\neq 0$ only for $t - t' > 0$, and is equal to

$$\mathcal{G}(x-x', t-t') = \frac{i}{2\pi} \int_{-\infty}^{+\infty} dk\, \frac{e^{i\,k((x-x')-c(t-t'))} - e^{i\,k((x-x')+c(t-t'))}}{2\,c\,k} \tag{68}$$

Further calculation

By symmetry in $k \to -k$ (68) becomes:

$$\frac{1}{4\pi\, c}\int_{-\infty}^{+\infty} dk\, \frac{\sin\left(k[(x-x')-c(t-t')]\right)-\sin\left(k[(x-x')+c(t-t')]\right)}{k} =$$

$$\frac{1}{4\, c}\left(\mathrm{sign}\left([(x-x')+c(t-t')]\right)-\mathrm{sign}\left([(x-x')-c(t-t')]\right)\right),$$

where $\mathrm{sign}(A)=1$, if $A>0$; $=-1$, if $A<0$; $=0$, if $A=0$.
The last integral is calculated in the complex k-plane as the real part of $\int_{-\infty}^{\infty} dk\, \frac{e^{ikA}}{k}$.
The Green's function is $\mathcal{G}(x-x', t-t') = \frac{1}{2\, c}$, if $t>t'$, and $-c(t-t') < (x-x') < c(t-t')$, and zero otherwise.
Nonzero response only in the part of the $(t,\, x)$- plane between the characteristics $x \pm c\, t$ $\leftrightarrow$ no response faster then the speed of waves c.