Discretization of Laplacian Operator

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Objetive of the presentation

In this presentation we want to show how to discretize the Laplacian operator through rectangular and triangular meshes, and as this allows to solve differential equations in partial derivatives through of systems of linear equations. An example is given about the solution of the heat equation in the one-dimensional and two-dimensional cases, and the Poisson equation using the Galerkin approximation.

Later we will explain what is the Heat Method to find the geodesic distance in general manifolds, and we will show how we want to articulate this method to the diffusion kernels that we have studied previously.

Introduction

Let u be a real function of three variables, $u = u(x, y, z)$, the **Gradient** of this function represents a vector field given by

$$\nabla u = \frac{\partial u}{\partial x} i + \frac{\partial u}{\partial y} j + \frac{\partial u}{\partial z} k = X \ ,$$

while its **Divergence** and its **Laplacian** are scalar fields expressed as

$$\Delta u = \frac{\partial^2 u}{\partial^2 x} + \frac{\partial^2 u}{\partial^2 y} + \frac{\partial^2 u}{\partial^2 z} = \nabla \cdot X = \nabla \cdot (\nabla u) \ .$$

The expression $\Delta u = \nabla \cdot (\nabla u)$ is not always fulfilled, for this we resort to the generalization of this operator known as Laplace-Beltrami and given by equality

$$\Delta_g u = \frac{1}{\sqrt{\det g}} \sum_j \frac{\partial}{\partial x_j} \left(\sum_i g^{ij} \sqrt{\det g} \frac{\partial u}{\partial x_i} \right) \ , \qquad (1)$$

where g is the metric associated with the coordinates $(x_1, x_2, \ldots, x_n)$ in the manifold.

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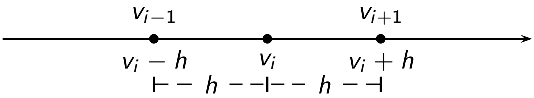
3. Heat equation: $\Delta u = \alpha \frac{\partial u}{\partial t}$. In problems of: heat transfer.
4. Wave equation: $\Delta u = \frac{1}{c^2} \frac{\partial^2 u}{\partial t^2}$. In problems of: acoustics, quantum mechanics.

Laplacian operator in one dimension

Consider a function $u(x)$ of a variable with derivatives of all orders. Let v_i be a given point and h an increase in both directions, it will be denoted by $u_i = u(v_i)$, $u_{i+1} = u(v_i + h)$ y $u_{i-1} = u(v_i - h)$.



From Tylor's serie is posible to express a function as a linear combination of its derivates through

$$u\left(v_{i+1}\right) \approx u(v_i) + u^{(1)}(v_i)h + \frac{1}{2}u^{(2)}(v_i)h^2 + \frac{1}{6}u^{(3)}(v_i)h^3 + \frac{1}{24}u^{(4)}(v_i)h^4 \ ,$$

$$u\left(v_{i-1}\right) \approx u(v_i) - u^{(1)}(v_i)h + \frac{1}{2}u^{(2)}(v_i)h^2 - \frac{1}{6}u^{(3)}(v_i)h^3 + \frac{1}{24}u^{(4)}(v_i)h^4 \ .$$

Laplacian operator in one dimension

Subtracting and adding both expressions it is possible to conclude equalities

$$u'(v_i) = \frac{1}{2h}\left[u(v_{i+1}) - u(v_{i-1})\right] + o(h^3)\ .$$

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There are alternative equations to discretize the first derivative by means of this method called **Finite Differences**. Two alternative expressions are

$$u'(v_i) = \underbrace{\frac{1}{h}\left[u(v_{i+1}) - u(v_i)\right]}_{\text{difference forward}} \quad \text{y} \quad u'(v_i) = \underbrace{\frac{1}{h}\left[u(v_i) - u(v_{i-1})\right]}_{\text{difference backward}}\ .$$

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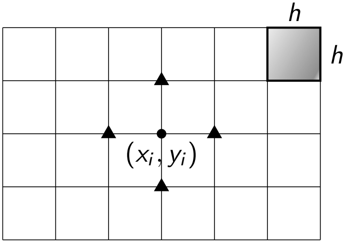
Laplacian operator for a function of one variable is written as

$$(\Delta u)_{v_i} = \frac{1}{h^2}\sum_{j\sim i}\left(u(v_j) - u(v_i)\right)\ , \qquad (2)$$

where $j \sim i$ means neighboring vertices to v_i.

Laplacian operator in a rectangular mesh

If the function is of two variables let us say $u = u(x, y)$ then Laplacian is the sum of the partial derivatives of order 2 for the two variables, in this case, Laplacian operator at a point $v_i = (x_i, y_i)$ is of the form



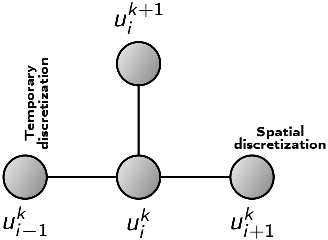
$$(\Delta u)_{v_i} = \frac{1}{h^2}\left[u(x_{i+1}, y_i) + u(x_{i-1}, y_i) + u(x_i, y_{i-1}) + u(x_i, y_{i+1}) - 4u(x_i, y_i)\right] \ ,$$

$$(\Delta u)_{v_i} = \underbrace{\frac{1}{h^2}}_{weight} \sum_{j \sim i} (u(v_j) - u(v_i)) \ .$$

The term h^2 represents the area of each of the squares in the rectangular mesh, however the increments in x and in y may be differents.

Heat equation can be defined as $\frac{\partial u}{\partial t} = \alpha \Delta u$ where α is a constant called **diffusivity** of the material, while u is the temperature distribution for a specific position and times. In the expression u_i^k the subscript indicates the position in the bar (the vertex) and the superscript the temporal moment

Bar: If we consider a bar of length L (with steps of h units) and Δt the discretization of time, then the solution for finite differences is written as



$$u_i^{k+1} = r\left(u_{i+1}^k + u_{i-1}^k\right) + (1-2r)u_i^k \quad \text{where } r = \frac{\alpha \Delta t}{h^2}\,. \qquad (3)$$

For the solution to be convergent to the theoretical solution it is necessary that $0 < 1 - 2r < 1$ in that case, $\Delta t < \frac{h^2}{2\alpha}$, so the choice of temporal discretization is not arbitrary.

Example 1 in one dimension

Consider a bar of length L, the heat equation defined on it with conditions of border and initials is given by

$$\begin{cases} u_t = \alpha u_{xx}, \\ u(L,t) = 0 \quad \text{for all } t > 0, \\ u(0,t) = 0 \quad \text{for all } t > 0, \\ u(x,0) = f(x) = x(L-x) \quad \text{for all } x \in [0,L] \,. \end{cases}$$

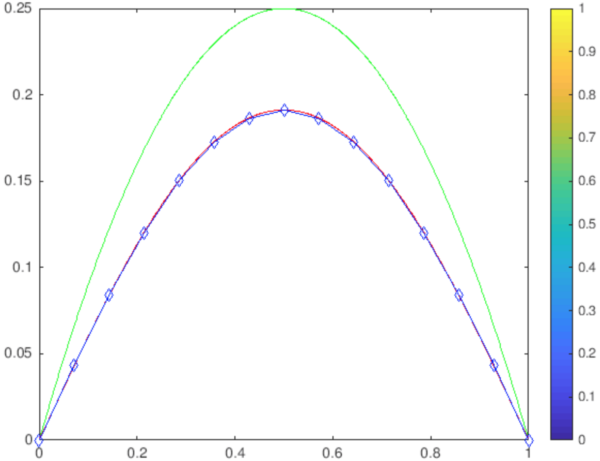
Analytical solution by separation of variables is

$$u(x,t) = \sum_{n=1}^{\infty} \frac{8L^2}{\pi^3(2n-1)^3} \exp\left(-\frac{\alpha(2n-1)^2\pi^2}{L^2}t\right) \sin\left(\frac{(2n-1)\pi}{L}x\right) \,. \tag{4}$$

For the simulation, $L = 1$ and $\alpha = 0.001$ were assumed.

Example 1 in one dimension

Green line represents the function $f(x) = x(L - x)$ of the initial condition. Blue line with the diamonds represents the approximate solution with the finite differences and the red line is the analytical solution, both for a time $t = 30$.



In this second example, again we will take the bar length L and the conditions

$$\begin{cases} u_t = \alpha u_{xx}, \\ u(L,t) = 100 \quad \text{for all } t > 0, \\ u(0,t) = 0 \quad \text{for all } t > 0, \\ u(x,0) = 0 \quad \text{for all } x \in [0,L] . \end{cases}$$

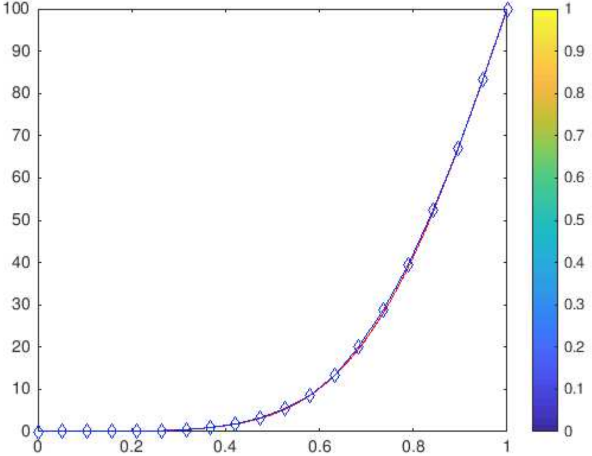
The analytical solution of this system is

$$u(x,t) = \frac{100}{L}x + \sum_{n=1}^{\infty} \frac{200}{n\pi}\cos(n\pi)\exp\left(-\frac{\alpha n^2\pi^2}{L^2}t\right)\sin\left(\frac{n\pi}{L}x\right) . \quad (5)$$

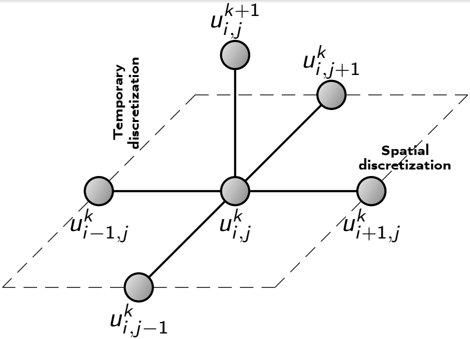
For the simulation, $L = 1$ and $\alpha = 0.001$ were assumed.

Example 2 in one dimension

Green line represents the function $f(x) = x(L - x)$ of the initial condition. Blue line with the diamonds represents the approximate solution with the finite differences and the red line is the analytical solution, both for a time $t = 30$.



Heat equation in two dimensions



Lamina: When we consider a rectangular sheet, the solution to the heat equation by finite difference is written as

$$u_{i,j}^{k+1} = r_x^2\left(u_{i+1,j}^k + u_{i-1,j}^k\right) + r_y^2\left(u_{i,j+1}^k + u_{i,j-1}^k\right) + \left(1 - 2r_x^2 - r_y^2\right)u_{i,j}^k\,, \tag{6}$$

where $r_x = \frac{\alpha\Delta t}{\Delta^2 x}$ and $r_y = \frac{\alpha\Delta t}{\Delta^2 y}$. For the solution to be stable, it must be fulfilled $\Delta t < \frac{1}{4\alpha}\left(\Delta^2 x + \Delta^2 y\right)$.

Example 3 in two dimensions

Consider a thin sheet that measures $L \times M$, the heat equation with boundary and initial conditions on it are defined as

$$\begin{cases} u_t = \alpha \left(u_{xx} + u_{yy} \right) \ , \\ u(x,0,t) = 0 \quad \text{for all } x \in [0,L] \text{ and } t > 0 \ , \\ u(x,M,t) = 0 \quad \text{for all } x \in [0,L] \text{ and } t > 0 \ , \\ u(0,y,t) = 0 \quad \text{for all } y \in [0,M] \text{ and } t > 0 \ , \\ u(L,y,t) = 0 \quad \text{for all } y \in [0,M] \text{ and } t > 0 \ , \\ u(x,y,0) = xy(1-x)(1-y) \quad \text{for all } (x,y) \in [0,L] \times [0,M] \ . \end{cases}$$

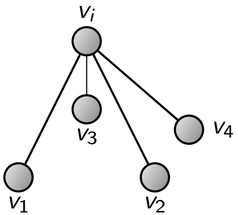
The analytical solution of this system is

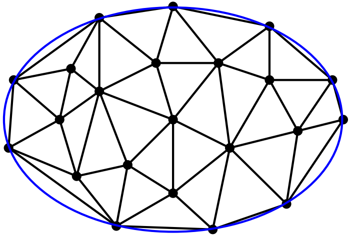
$$u(x,y,t) = \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} c_{mn} \exp\left(-\alpha \left(\frac{m^2\pi^2}{L^2} + \frac{n^2\pi^2}{M^2} \right) t \right) \sin\left(\frac{m\pi}{L} x \right) \sin\left(\frac{n\pi}{M} x \right) \tag{7}$$

where $c_{mn} = \frac{16L^2M^2}{m^3n^3\pi^6} \left(1 - (-1)^m\right)\left(1 - (-1)^n\right)$. For the simulation, $L = 1$, $M = 1$, and $\alpha = 0.001$ were assumed.

Laplacian in a triangular mesh

When the surface is not regular, it is easier to construct a mesh by means of triangles starting from $|V|$ vertices, where the edges can not be cut from each other. This way of doing the discretization allows whether the surface is flat or three-dimensional, where each vertex v_i is part of the manifold (surface).





In this situation, Laplacian Operator associated with a vertex v_i is written as

$$(Lu)_i = \sum_{j\sim i} w_{ij} \left(u_j - u_i\right) \ . \tag{8}$$

Galerkin's approach

First identity of Green is given by

$$\int_M g\Delta f \; dA = \oint_{\partial M} g \left(\nabla f \cdot n\right) \; ds - \int_M \left(\nabla g \cdot \nabla f\right) \; dA \,. \tag{9}$$

Let f be a function in the manifold M, this determines the operator $\mathcal{L}_f$ such that

$$\mathcal{L}_f[g] = \int_M fg \; dA \tag{10}$$

for every function g of an integrable square defined on M. The function g is called **test function**. If a compact surface without a border is considered, then $\partial M = \phi$ and the Green's identity allows us to write equality

$$\mathcal{L}_{\Delta f}[g] = -\int_M \left(\Delta f \cdot \Delta g\right) \; dA = \mathcal{L}_{\Delta g}[f] \,.$$

Poisson equation

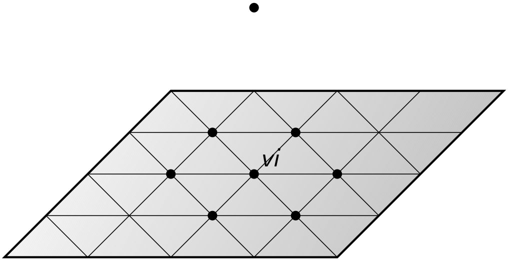
Consider the Poisson equation $\Delta u = g$ it can be written by the operator $\mathcal{L}$, or in its weak formulation, as $\mathcal{L}_{\Delta u}[\phi] = \mathcal{L}_g[\phi]$ that in its integral form is

$$\int_M \phi \Delta u \, dA = \int_M \phi \, g \, dA \, .$$

The function g is known in this approach. While the ϕ functions are the test functions. In the case of a triangular mesh these functions will be called **hat function**.

Hat function in a triangular mesh

In the case of triangular mesh of $|V|$ vertices denoted v_i, linear functions are chosen for sections denoted $h_i = h(v_i)$ and defined as 1 in the associated vertex and zero in the other vertices.



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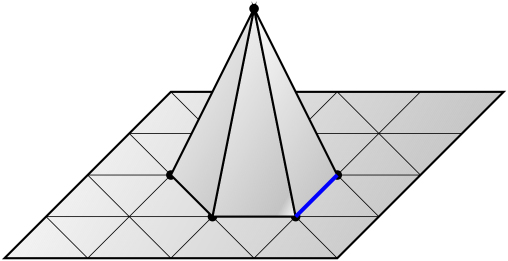


If $u(v_i)$ is expressed as a vector $\overrightarrow{a}$, where each component is the value of u in each vertex v_i then it can be approximated by means of equality

$$u(v) = \sum_{i=1}^{|V|} h_i a_i \ .$$

The values of g are known and can be written as the vector $\overrightarrow{b}$.

Poisson equation

With each h_i as a test function and by the Galerkin method the Poisson equation is written as

$$\int_M h_i \, \Delta u \, dA = \int_M h_i g \, dA \quad \text{for each } i = 1, 2, \ldots, |V|. \tag{11}$$

Because of Green's identity, the left side is written as

$$\int_M h_i \Delta u \, dA = -\int_M (\nabla h_i \cdot \nabla u) \ dA = -\sum_j a_j \int_M (\nabla h_i \cdot \nabla h_j) \ dA = \left(L_c \vec{a}\right)_i$$

where $L_c = [L_{ij}]$ is a matrix called **Laplacian cotangent** and whose components are

$$L_{ij} = \int_M (\nabla h_i \cdot \nabla h_j) \ dA \, . \tag{12}$$

Poisson equation

On the right side you have equality

$$\int_M h_i g \; dA = \sum_j b_j \int_M (h_i \cdot h_j) \; dA = \left(\mathrm{A}\overrightarrow{b}\right)_i$$

where $\mathrm{A} = [\mathrm{A}_{ij}]$ is the **Mass matrix** with components

$$\mathrm{A}_{ij} = \int_M (h_i \cdot h_j) \; dA \, . \tag{13}$$

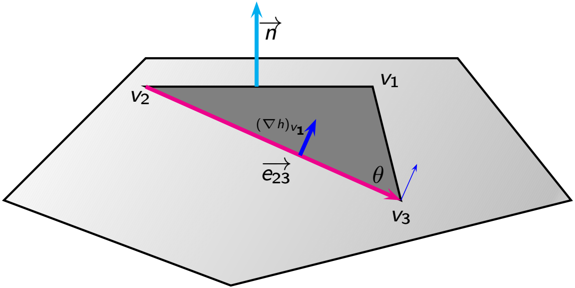
Poisson equation is written as a system of linear equations of the form

$$L_c \overrightarrow{a} = \mathrm{A}\overrightarrow{b} \quad \text{equivalent to} \quad \underbrace{\left(\mathrm{A}^{-1} L_c\right)}_{\text{Laplacian operator}} \overrightarrow{a} = \overrightarrow{b} \, . \tag{14}$$

Since h_i is a linear function by sections in each triangular face then ∇h_i is constant and is also orthogonal to a normal unitary vector $\overrightarrow{n}$ to the face. Consider a triangle with vertices v_1, v_2 and v_3. For h_i the expression is satisfied $h(v) - h(v_0) = \nabla h \mid_{v_0} \cdot (v - v_0)$ where the following conclusions are obtained:

- $(\nabla h)_{v_1}$ is orthogonal to edge $v_2 v_3$,
- $\|(\nabla h)_{v_1}\| = \frac{1}{h}$.

where h is the height of the triangle relative to the vertex v_1. Each vector $(\nabla u)_{v_i}$ lies in the plane that contains the triangle



The magnitude of this vector can also be written $\|(\nabla h)_{v_1}\| = \frac{1}{2A}\left\|\overrightarrow{e_{23}}\right\|$ where $\mathcal{A}$ is the area of the triangular face. The gradient associated with the vertex v_1 is written as

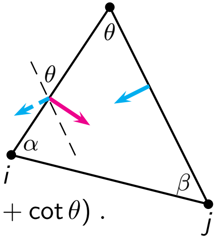
$$(\nabla h)_{v_1} = \frac{1}{2\mathcal{A}}\left(\overrightarrow{n} \times \overrightarrow{e_{23}}\right) \ . \tag{15}$$

While the gradient associated with the triangular face is given by

$$\nabla h = \frac{1}{2\mathcal{A}}\sum_{i=1}^{3}\left(\overrightarrow{n} \times \overrightarrow{e_i}\right) \tag{16}$$

where $\overrightarrow{e}_i$ is the vector associated with the edge.

Since we know the gradient associated with each vertex of a triangular face, it is now necessary to know the value of the scalar product between two of these vectors.



Case I: Two functions h_i and h_j are defined in the same vertex, in this case $h_i = h_j$. With this condition it is shown that

$$\int_T (\nabla h_i \cdot \nabla h_i)\ dA = \mathcal{A}\|\nabla h_\alpha\|^2 = \frac{1}{2}(\cot\beta + \cot\theta)\ .$$

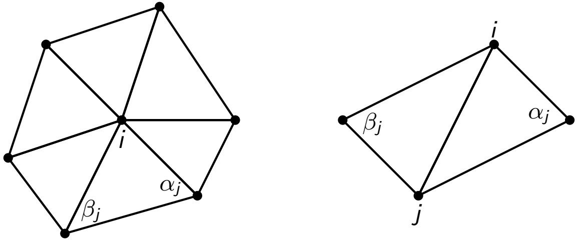
Case II: Functions h_i and h_j are defined on vertices different but that share the same edge. In that case we have

$$\int_T (\nabla h_\alpha, \nabla h_\beta)\ dA = \mathcal{A}\,(\nabla h_\alpha, \nabla h_\beta)$$

$$= \mathcal{A}\,\|\nabla h_\alpha\|\,\|\nabla h_\beta\|\cos(180^\circ - \theta) = -\frac{1}{2}\cot\theta\ .$$

Applying this to the whole triangular mesh, we have that the Laplacian cotangent matrix is given by

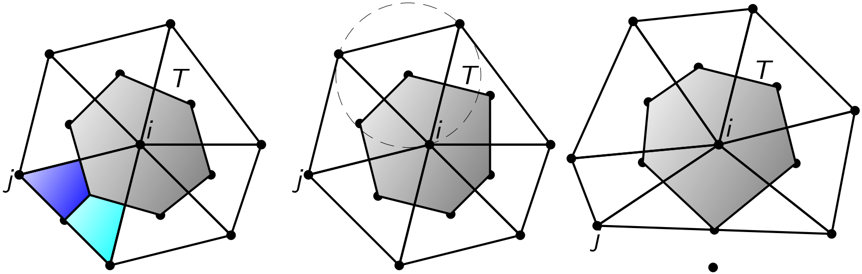
$$(L_c)_{ij} = \begin{cases} \frac{1}{2} \sum_{k \sim i} (\cot \alpha_k + \cot \beta_k) & \text{if } i = j \\ -\frac{1}{2} (\cot \alpha_j + \cot \beta_j) & \text{if } j \sim i \\ 0 & \text{otherwise} \end{cases} . \tag{17}$$



Mass matrix

Mass matrix is a diagonal matrix where the components of the main diagonal can be found by any of the following methods:

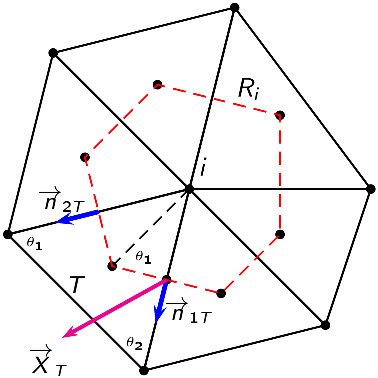
Case I: Through the barycenters.
Case II: Through the circumcenters.
Case III: A mixed case between the circumcenters of the triangles with an angle $\theta < \frac{\pi}{2}$ and the midpoint of the edge opposite the angle when it measures more than one right angle.



The use of one method or another depends on the application. If we use the idea of the barycenter, the components are a third of the area of the triangle that they indicate in the vertex i.

Divergence in a triangular mesh

Let X be a vector field that acts on each face of the triangular mesh. Let R_i be the region formed by the circumcenters of each triangle T determined by the neighbors at the vertex i.



Where $\overrightarrow{n_{1T}}$ is a unit vector external to the closed region R_i acting on the direction of the edge $\overrightarrow{e_{1T}}$, also with $\overrightarrow{n_{2T}}$ in respect of $\overrightarrow{e_{2T}}$. And $\overrightarrow{X_T}$ is the X component that acts on the triangular face T.

Divergence in a triangular mesh

By the Stokes Theorem applied to this closed region we have

$$\int_{R_i} \nabla \cdot X \, dA = \int_{\partial R_i} \overrightarrow{X} \cdot \overrightarrow{n} \, d\ell = \sum_T \left[\int_{l_{\mathbf{1}T}} \overrightarrow{X_T} \cdot \overrightarrow{n_{1T}} \, d\ell + \int_{l_{\mathbf{2}T}} \overrightarrow{X_T} \cdot \overrightarrow{n_{2T}} \, d\ell \right] .$$

Since $\overrightarrow{n_{1T}}$ is a unit vector in the same direction as the edge $\overrightarrow{e_{1T}}$ it is written $\overrightarrow{X_T} \cdot \overrightarrow{n_{1T}} = \frac{1}{\|e_{\mathbf{1}T}\|} \left(\overrightarrow{X_T} \cdot \overrightarrow{e_{1T}} \right)$. According to the trigonometric ratios we have

$$\cot(\theta_1) = \frac{2l_{1t}}{\|e_{1T}\|} \quad \text{equivalent to} \quad \frac{1}{\|e_{1T}\|} = \frac{\cot(\theta_1)}{2l_{1T}} .$$

Which implies that the scalar product $\overrightarrow{X_T} \cdot \overrightarrow{n_{1T}} = \frac{1}{2l_{\mathbf{1}T}} \cot(\theta_1) \left(\overrightarrow{X_T} \cdot \overrightarrow{e_{1T}} \right)$ is constant with respect to each triangle and it turns out that

$$\int_{R_i} \nabla \cdot X \, dA = \sum_T \frac{1}{2} \left[\cot(\theta_1) \left(\overrightarrow{X_T} \cdot \overrightarrow{e_{1T}} \right) + \cot(\theta_2) \left(\overrightarrow{X_T} \cdot \overrightarrow{e_{2T}} \right) \right] \quad (18)$$

where e_{1T} and e_{2T} vary on the same sides of a triangle for each fixed vertex i.

The problem of Geodesic distance

Let ϕ be a function defined in M and X a vector field. The functional $E[\cdot]$ on the manifold is defined as

$$E[\phi] = \int_M \|\nabla\phi - X\|^2 \; dA \, .$$

It is possible to demonstrate that this functional is convex and therefore must have a minimum, by the first identity of Green, it is possible to demonstrate that

$$E[\phi] = -\langle \phi, \Delta\phi \rangle + \langle \phi, \nabla \cdot X \rangle + \langle X, X \rangle \, .$$

For this functional the derivative is defined as

$$D_\psi E[\phi] = \lim_{\epsilon \to 0} \frac{E[\phi + \epsilon\psi] - E[\phi]}{\epsilon}$$

whose gradient is $\nabla E[\phi] = 2\nabla \cdot X - 2\Delta\phi$ and finally said gradient is zero (the minimum) when

$$\Delta\phi = \nabla \cdot X \, . \qquad \text{(Poisson equation)} \tag{19}$$

Heat method

This method was presented by Keenan Crane, which allows to calculate the geodesic distance ϕ on a manifold through of heat equation. It involves three steps namely:

Step I: Solve the heat equation $\frac{\partial u}{\partial t} = \Delta u$. Doing a **discretization of time** results

$$\frac{u_t - u_0}{t} = \Delta u_t \quad \text{from where} \quad (Id - t\Delta)u_t = u_0 \ ,$$

where u_0 is the inicial condition on a vertex i (Dirac delta). If we consider the Laplacian operator as the product of the inverse of the mass matrix with the cotangent operator (**spatial discretization**), then we have $\Delta = L = \mathrm{A}^{-1}L_c$ and therefore the previous equation write as

$$\left(\mathrm{A} - tL_c\right) u_t = \mathrm{A} u_o = \delta \ , \tag{20}$$

which is a system of linear equations whose solution u_t is the distribution of temperatures in **each vertex** after a time t.

Step II: Evaluate vector field $X = -\frac{1}{\|\nabla u\|}\nabla u$ by **each face**. With the solution obtained for u_t in the previous step, we get an expression for the gradient by means of equality

$$(\nabla u)_f = \frac{1}{2\mathcal{A}_f}\sum_{i=1}^{3} u_i \left(\overrightarrow{n} \times \overrightarrow{e_i}\right) \tag{21}$$

where $\mathcal{A}_f$ is the triangular face area, $\overrightarrow{n}$ is a normal unit on that face, and u_i is the value of u_t at the vertex i.

Heat method

Step III: Solve the Poisson equation $\Delta\phi = \nabla \cdot X$. Known vector field X in step II, its divergence is given by

$$\nabla \cdot X = \frac{1}{2}\sum_j \left[\cot(\theta_1)\left(\overrightarrow{X_j} \cdot \overrightarrow{e_1}\right) + \cot(\theta_2)\left(\overrightarrow{X_j} \cdot \overrightarrow{e_2}\right)\right] . \qquad (22)$$

This divergence is calculated for **each vertex**. Poisson equation can be solved by means of the Galerkin approximation whose solution is of the type $\left(\mathrm{A}^{-1}L_c\right)\overrightarrow{a} = \overrightarrow{b}$ where $b = \Delta \cdot X$.

Interest in this method

Why are we interested in this Method?

We are interested in finding Diffusion Kernels that fit a family of probability distributions that model a data set. These kernels are obtained with the objective of making classification on this set of supervised data.

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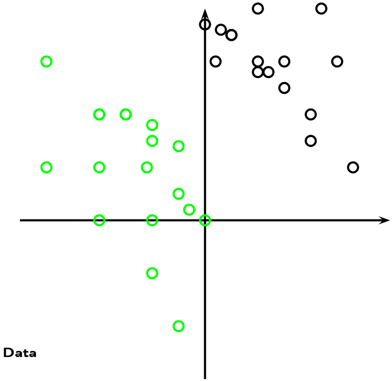

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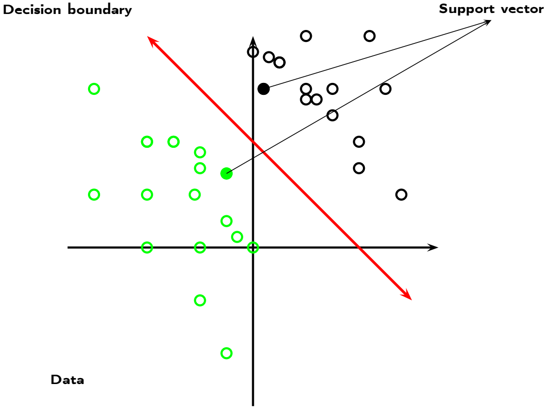

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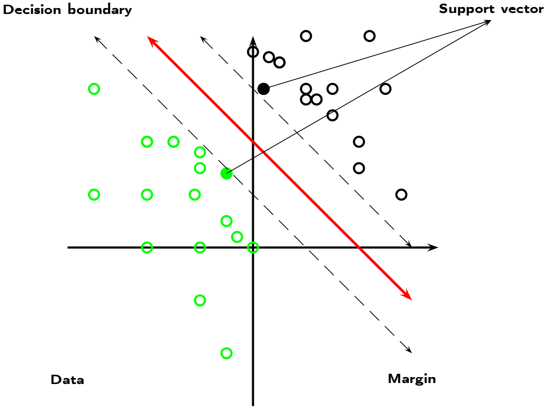

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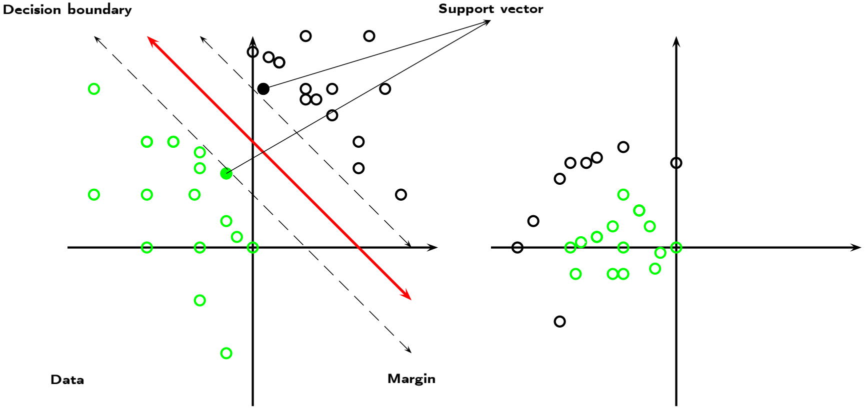

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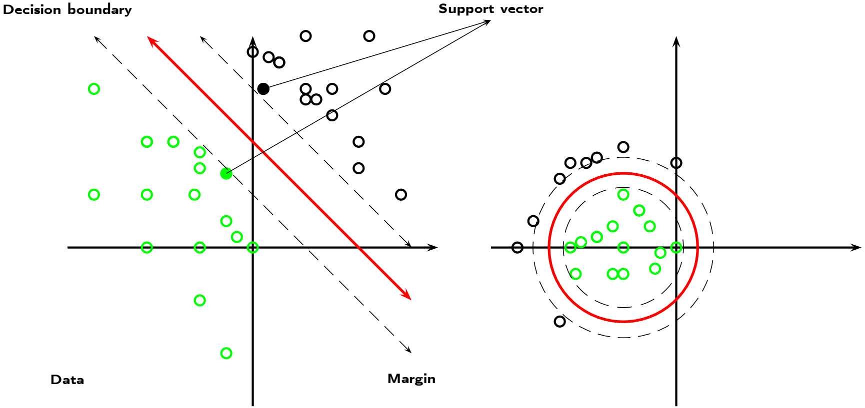
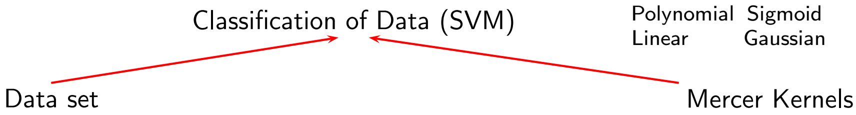
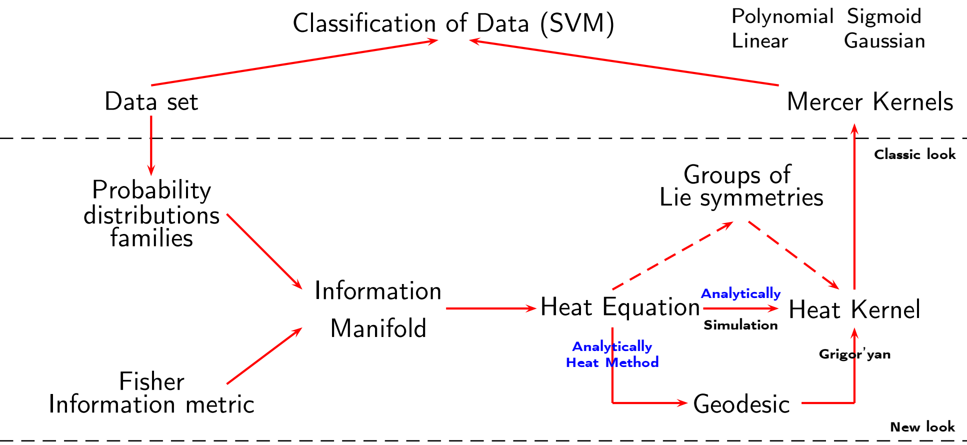


Diffusion kernels in SVM



Classic look

Diffusion kernels in SVM



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Thank you!!