Zero Crossings and the Heat Equation

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Abstract

We analyze the "zero crossings" of a solution to the heat equation. Zero crossings of differences of multiple levels of resolution of data have been used for representation and analysis of digitized signals and images. We establish a mathematical structure, based on the heat equation, for investigating these kinds of representations. We show that zero crossings are surfaces which evolve in time, and that no new zero crossing surfaces appear at positive values of time. We show that complete knowledge of the zero crossings of a solution to the heat equation, together with gradient data at those zero crossings, uniquely determines the initial data. We provide an algorithm, via the backwards heat equation, for reconstructing the initial data given the zero crossings and gradient. We argue that, in general, the zero crossings alone are insufficient to determine the initial data.

I. The Heat Equation for Multiresolution Representation

It is increasingly clear that the use of multi-resolution representation is an important idea for the analysis of signal and image data. Many data structures have been studied, including "gaussian pyramids," difference of gaussian channels, and Laplacian pyramids [1,2,3]. The goal of these decompositions of scalar data is the representation of essential information in a scale invariant fashion permitting easy feature extraction and matching with models. We show below that these structures may be studied by means of a unifying mathematical treatment based on the heat equation. We then define the notion of zero-crossings, and discuss their significance.

Let f(x) be a bounded function defined for $x \in \mathbb{R}^n$. If we blur f(x) by increasingly diffuse gaussians parameterized by t>0, we obtain

$$u(x,t) = \int_{\mathbb{R}^n} K(x-y,t)f(y)dy , \qquad (1.1)$$

where

$$K(x,t) = (4\pi t)^{-n/2} e^{-|x|^2/4t}$$
, (1.2)

K(x,t) is the fundamental solution to the heat equation; in fact, u(x,t) can be shown to be the unique bounded solution to the initial value heat equation:

$$u_t = \Delta u , \qquad (1.3)$$

$$u(x,0) = f(x)$$
 (1.4)

Next, consider $v(x,t) = \Delta u(x,t)$. The function v is itself a

solution to the heat equation, and can be interpreted in three ways. First, by definition,

$$v(x,t) = \Delta u(x,t) = u_t(x,t)$$
.

Second, by standard calculus of convolutions,

$$v(x,t) = \int_{\mathbb{R}^n} \Delta K(x-y,t) f(y) dy . \qquad (1.6)$$

Here we think of v(x,t) as a filtered version of f(x), using the filter $\Delta K(x,t)$, i.e., the laplacian of a gaussian. The kernel ΔK can be viewed as a bandpass filter, and is frequently modeled as the difference of two gaussians. The model is logical, since K(x,t) is itself a solution to the heat equation, and thus

$$\Delta K(x,t) = K_t(x,t) \approx 1/\epsilon (K(x,t+\epsilon) - K(x,t)) .$$

Using the first interpretation of v(x,t) note that

$$-\int_{0}^{\infty} v(x,t)dt = -\int_{0}^{\infty} u_{t}(x,t)dt = f(x)$$
 (1.7)

provided that $u(x,t) \neq 0$ as $t \neq \infty$. (It is sufficient, for example that $f \in L^1$). Thus f(x) can be reconstructed from v(x,t).

The second interpretation views v(x,t) as a solution to the initial value heat equation using initial data $g(x) = \Delta f(x)$. We see that complete knowledge of v(x,t) is assured in any representation from which one can reconstruct g(x). Once v(x,t) is determined, then f(x) (and also u(x,t)) are also specified, according to Equation (1.7).

Thus a representation of the v(x,t) data provides an implicit representation of the f(x) and u(x,t) data. Since v(x,t) is a solution to the heat equation, we are henceforth concerned with representations of the data in a solution to the heat equation such that some form of the initial data can be reconstructed. In what follows, u(x,t) will stand for any generic solution to the heat equation, with f(x) as initial data, although in terms of the above notation, v(x,t) and g(x) are likely instances of the representation problem.

So consider a solution u(x,t) to the heat equation defined in the space $\{(x,t)|x\in\mathbb{R}^n,t\geq 0\}$. The zero set of u(x,t) is the point set in (x,t) where u=0. This set might be empty (for instance, if f is subharmonic or superharmonic), everything (if f(x) is harmonic), or a proper subset of (x,t) space. In the latter case, the zeros can be isolated points, lines, and surfaces (but never regions). However, components of the zero set which are isolated points and lines of codimension greater than one are degenerate, in the sense that u will be nonnegative (or nonpositive) in a region of any point of the component. Components of the zero set which separate positive and negative regions will be surfaces, and have a special definition:

Definition:

The zero crossings refer to the surfaces separating regions where a function is positive and where it is negative. For a solution u(x,t) to the heat equation, the zero crossings refer to the point set

 $\partial \{(x,t)|u(x,t)>0\} \cap \partial \{(x,t)|u(x,t)<0\}.$

Since u(x,t) is a smooth function for t>0 (analytic, in fact), the zero crossings will necessarily be a collection of surfaces of codimension one, analytic except possibly for discrete cusps, satisfying u=0 on the surfaces.

For imagery data, it has been argued that the zero crossings of a laplacian of a gaussian filter $(\Delta K(x,t))$ of the image data include all edges of significance at the corresponding level of resolution [4], and accordingly might be associated with human visual neural processing of retinal intensity data [5]. Zero crossings have also been used as features for stereo matching and motion correspondence between pairs of images (e.g., see [6]).

It is clear that any nonzero scalar multiple of a solution u(x,t) will have an identical set of zero crossings as u(x,t). It has been recognized, at least intuitively, that zero-crossings alone do not contain all the information in the initial data, even modulo a scalar factor, but that zero crossings together with slope information should permit reconstruction [7]. Lack of a theoretical foundation has been lamented. We show here that these intuitions were correct, and that the theory is quite simple.

If we consider a representation to be a map from one topological space to a (hopefully simpler) topological space, the value of the representation can be determined by analyzing the <u>fibers</u> of the map and the preimage of local neighborhoods. A fiber of the map is the set of elements which map to a single element or representation. Generally, a useful representation will map many elements to a single element, but that the class of elements in a fiber share properties which are essential to the interpretation of those objects. The stability of the

representation, however, is a separate matter. Since the representation of an element can never be presented with infinite precision, the preimage of a local neighborhood of a representation is the true collection of elements represented. Both issues need to be analyzed for the proposal to represent signal and image data by zero-crossings of bandpass filters of the data. Our results in the following sections are intended as initial investigations along these lines.

II. Consequences of the Maximum Principle

In this section, we show that the maximum principle for parabolic equations implies that zero crossings are never created as t increases. We further show, using the Hopf maximum principle, that there exists at most one solution of the heat equation with specified zero crossings and specified gradient data at those zero crossings. The first result has been discussed in the context of data representation in artificial intelligence [8] (at least for n = 1), but to our knowledge previous treatments were independent of the maximum principle.

Let u(x,t), $x \in \mathbb{R}^n$, t > 0 be a nonzero bounded solution to heat equation, and let A denote its zero crossings. The zero crossing surfaces will evolve as t increases, but according to the theorem below, no surface can be completely separated from the initial hyperplane $\{t=0\}$:

Theorem 2.1: A component of A is a surface which starts at the hyperplane $\{t = 0\}$, and either ends at the hyperplane $\{t = 0\}$ or extends to infinity.

Note that for n = 1, the zero crossings are curves. In general, the surfaces of A admit local real analytic parameterizations, and therefore have at most isolated cusp singularities. The content of Theorem 2.1 can be summarized as $\partial A \subseteq \{t=0\}$. Before proving the theorem, we state our second result:

Theorem 2.2: Suppose we are given a collection of surfaces A (consistent with Theorem 2.1) and specified gradient data on A. Then

there exists at most one solution u(x,t) to the heat equation having A as its zero crossings and the specified gradient data on A.

Thus given the zero crossings and gradient data on those zero crossings of a solution u(x,t) to the heat equation, then u(x,t) is uniquely specified, and there is no other solution having simultaneously the same zero crossing surfaces and gradient data on those surfaces. In particular, the initial data f(x) = u(x,0) is uniquely specified by the zero crossing and gradient data. The solution u(x,t), provided it exists, can be constructed by the algorithm presented in Section III.

Theorem 2.1 and 2.2 follow easily from versions of the maximum principle for parabolic partial differential equations. For completeness, we state these theorems in a general form useful for us:

Theorem 2.3 [as stated in 9]:

Let D be a domain of the (n+1)-dimensional (x,t) space, and suppose that $\Delta u - u_t > 0$ in D. Suppose that the maximum of u(x,t) in D is obtained at an interior point $(x_0,t_0) \in D$, with $u(x_0,t_0) = M$. Then $u(x_1,t_1) \equiv M$ at all points $(x_1,t_1) \in D$ which can be connected to (x_0,t_0) by a path in D consisting only of horizontal and vertical segments.

Theorem 2.4. A Hopf boundary lemma for parabolic equations [9]. As in Theorem 2.3, suppose that $\Delta u - u_t > 0$ in a domain D. Suppose that the maximum M of u(x,t) in D is attained at a point $P \in \partial D$. Assume that an (n+1) dimensional sphere in (x,t) space can be constructed such that P

lies on the boundary of the sphere, and the interior of the sphere lies entirely in D, with u < M in the sphere. Also suppose that the radial direction from the center of the sphere to P is not parallel to the t-axis. Then if $\frac{\partial u}{\partial v}$ denotes any directional derivative in an outward direction on ∂D , we have

$$\frac{\partial u}{\partial v} > 0$$
 at P.

Proof of Theorem 2.1: If a component of the zero crossing surfaces A encloses a region D separated from the hyperplane $\{t = 0\}$, then D is an open domain with u = 0 on ∂D . Either u or -u (also a solution to the heat equation) will contain a positive maximum attained at a point (x_0,t_0) in the interior of D. Since (x_0,t_0) can be connected to some point of a bounding zero crossing surface by a path whose interior lies in D, consisting of vertical and horizontal segments, thus Theorem 2.3 is violated.

<u>Proof</u> of <u>Theorem 2.2</u>: Suppose u(x,t) and v(x,t) are distinct solutions to the heat equation having identical zero crossing sets A and identical gradients on A. Then w(x,t) = u(x,t)-v(x,t) is also a solution to heat equation, vanishes on A, and has zero gradients on A. Now, the zeros of w are discrete surfaces and points which include A. Further, A consists of real analytic surfaces with possibly discrete cusps. Thus there exists some $P \in A$ so that a sphere can be constructed through P lying entirely on one side of the surface of A on which P lies, chosen sufficiently small so that w is strictly positive (or strictly negative) inside the sphere, and finally such that the center

of the ball is not directly above or below P. Since w = 0 at P, either w or -w has a maximum in the closed sphere at P. By Theorem 2.3, $\frac{\partial w}{\partial v} \neq 0$ at P, in any outward direction. This contradicts the fact that w(x,t) has zero gradient data at P.

All of the theorems in this section hold for a more general class of parabolic initial value problems, i.e.,

$$u_{+} = Lu \tag{2.1}$$

$$u(x,0) = f(x) \tag{2.2}$$

where

$$L = \sum_{i,j=1}^{n} a_{ij}(x,t) \frac{\partial^{2}}{\partial x_{i} \partial x_{j}} + \sum_{j=1}^{n} b_{j}(x,t) \frac{\partial}{\partial x_{j}}$$

is a strongly elliptic operator with bounded coefficients. In analogy with Equation (1.1), the solution to (2.4), (2.5) can be written as

$$u(x,t) = \int_{\mathbb{R}^n} G(x,t;y,0)f(y)dy \qquad (2.3)$$

where $G(x,t;y,\tau)$, $\tau \le t$ is the Green's function of the parabolic equation (2.4). The heat equation (1.3) is special in that its Green's function $K(x-y,t-\tau)$ (see (1.2)) depends only on |x-y| and $t-\tau$. Thus the solution to the heat equation problem (1.3), (1.4) is given by a radially symmetric convolution, in agreement with our intuitive notions of blurring and representation at lower resolution.

III. Reconstruction from the Zero Crossings and Gradient Data.

Suppose we are given the zero crossing set A, and the gradient data for a solution to the heat equation. In this section, we show how to reconstruct the solution u(x,t).

First, consider a component of A which encloses a bounded region D of the (x,t) half-space. The boundary of D consists of zero crossings $\Gamma \subseteq A$, and a portion Σ of the $\{t=0\}$ hyperplane: $\partial D = \Gamma \cup \Sigma$. Fix $y \in \mathbb{R}^n$ and $\tau > 0$, with τ greater than the range of t in D. Let

$$v(x,t) = K(x-y,\tau-t),$$
 (3.1)

and observe that

$$v_{+} + \Delta v = 0 \quad \text{in} \quad D. \tag{3.2}$$

We use the heat equation for u and Green's theorem to write

$$0 = \iint\limits_{D} (u_{t} - \Delta u)v + (v_{t} + \Delta v)u \, dxdt$$

$$= \iint\limits_{\partial D} [(uv)\xi + (u\nabla v - v\nabla u) \cdot \eta] d\sigma, \qquad (3.3)$$

where do is surface measure, and $(\eta,\xi)(x,t)$ is the outward pointing unit normal vector to ∂D at the point $(x,t) \in \partial D$, and $\nabla = \frac{\partial}{\partial x}$ refers to spatial derivatives only. Using the facts that $(\eta,\xi) = (0,-1)$ on Σ and u=0 on Γ , equation (3.3) becomes

$$\int_{(x,0)\in\Sigma} u(x,0)v(x,0)dx = -\int_{\Gamma} v(x,t)(\nabla u \cdot \eta)(x,t)d\sigma$$
 (3.4)

Let us define

$$\tilde{f}(x) = \begin{cases} f(x) & (x,0) \in \Sigma \\ 0 & (x,0) \notin \Sigma \end{cases}$$
(3.5)

and
$$\tilde{u}(x,t) = \int_{\mathbb{R}^n} K(x-z,t)\tilde{f}(z)dz$$
. (3.6)

Then equation (3.4) can be rewritten as

$$\tilde{u}(y,\tau) = \int_{\Gamma} K(x-y, \tau-t)(\nabla u \cdot \eta)(x,t) d\sigma$$
 (3.7)

Thus if we know Γ and the gradient of u along Γ , we can compute u(x,t) for $t > \max\{t \mid (x,t) \in D\}$. Since u(x,t) and f(x) are related by (3.6), we are in a situation where we want to reconstruct f(x) from u(x,t). This is achieved by solving the backwards heat equation. John [10], among many others, have considered algorithms to solve this problem. In general, a backsolution does not exist unless certain growth conditions are satisfied; in this case, the existence of a solution is guaranteed since f(x), given by (3.5), exists. From a numerical point of view, the construction of f(x) from u(x,t) is unstable. However, providing f(x) is sufficiently well behaved, since f(x) has compact support and is of constant sign, reasonable approximations to f(x) are in practice possible.

Once $\tilde{f}(x)$ is determined, then u is known on ∂D . Theoretically, then, u(x,t) can be determined in D, and then in all of (x,t)-space by analytic continuation. In practice, however, closer approximations will be obtained by treating each component bounded by A separately.

Since $\nabla u(x,t)$ on a zero crossing surface is always normal to the surface, the gradient data can be specified by a scalar function on A. According to equation (3.7), the most convenient form for the gradient data is $\nabla u \cdot \eta d\sigma$, where $\nabla u = (\frac{\partial u}{\partial x_1}, \dots, \frac{\partial u}{\partial x_n})$, and η is the horizontal component of the outward normal (η, ξ) . As an example, consider the special case n=1, and Γ given by t=t(x), |x| < a. In that case, (3.7) becomes

$$\tilde{u}(y,\tau) = \int_{-a}^{a} K(x-y, \tau-t(x)) \frac{\partial u}{\partial x}(x,t(x))t'(x)dx.$$

Note that this integral can be written in the form

$$u(y,\tau) = \int_{\Gamma} K(x-y, \tau-t) \frac{\partial u}{\partial x}(x,t)dt$$
,

where the integral is over all $(x,t) \in \Gamma$. A similar formula holds in higher dimensions.

However, the formula (3.7) applies only to the case where D is bounded. Next consider an unbounded component D of (x,t)-space with the zero crossing surfaces A removed. Let τ be greater than the range of t in all of the bounded components of (x,t) space less A. Finally, let $D_{\tau} = D \cap \{(x,t) | x \in \mathbb{R}^n, 0 < t < \tau\}$, see Figure 1.

We once again consider the integral in (3.3), this time integrating over D_{τ} . The boundary of this region consists of zero crossing surfaces Γ , portions $\Sigma \subseteq \{t=0\}$, and an additional boundary portion $\Sigma_{\tau} \subseteq \{t=\tau\}$. Analogous to (3.4), we obtain

$$\int_{(x,0)} u(x,0)v(x,0)dx + \int_{\Gamma} v(x,t)(\nabla u \cdot \eta)(x,t)d\sigma$$

$$(x,0) \in \Sigma$$

$$= \begin{cases} u(y,\tau) & (y,\tau) \in \Sigma_{\tau} \\ \\ 0 & (y,\tau) \notin \Sigma_{\tau} \end{cases}$$
 (3.8)

Here we have used the fact that $v(x,\tau) = K(x-y,0)$ is a delta function with mass at x = y. Define $\tilde{f}(x)$ and $\tilde{u}(x,t)$ as in (3.5), where Σ is now the $\{t=0\}$ portion of the boundary of the unbounded component D. In that case, (3.8) says

$$\tilde{\mathbf{u}}(\mathbf{y},\tau) = \int K(\mathbf{y}-\mathbf{x}, \tau-\mathbf{t})(\nabla \mathbf{u} \cdot \mathbf{\eta})(\mathbf{x},\mathbf{t}) d\sigma, \quad \text{for } (\mathbf{y},\tau) \notin \Sigma_{\tau}$$
 (3.9)

Since $u(y,\tau)$ is unknown, (3.8) gives no useful information when $(y,\tau) \in \Sigma_{\tau}$. To obtain the $u(y,\tau)$ data for $(y,\tau) \in \Sigma_{\tau}$, we must content ourselves with analytic continuation of the $u(y,\tau)$ for $(y,\tau) \notin \Sigma_{\tau}$, assisted by the fact that equation (3.9) holds with the unknown but small error $u(y,\tau)$ when $(y,\tau) \in \Sigma_{\tau}$. Once $u(y,\tau)$ has been extended in this manner for $y \in \mathbb{R}^n$, reconstruction of $\tilde{f}(x)$ is done by solving the backwards heat problem.

We are currently conducting numerical experiments to test the

feasibility and accuracy of these reconstructions for both bounded and unbounded regions enclosed by zero crossing surfaces.

IV. Representation using Zero Crossings Alone.

In this section, we sketch some ideas about the inverse problem that arises when the given data consists of the locations of the zero crossings, with no information about the gradient data. Obviously, the zero crossings of a function represents a class of functions that includes all scalar multiples of the original function. Thus reconstruction in this section refers to restoration to within a multiplicative constant.

We note that the zero sets of a function determine the function only in very special cases, i.e., if one has a very rich analytic structure such as complex analyticity. For example, a polynomial is determined (up to a multiplicative constant) by its degree and full set of zeros. Under certain conditions, the same is true for entire functions in the complex plane. In a more general situation, one has the celebrated Riemann Roch theorem of algebraic geometry. Logan's theorem [11] also is a uniqueness theorem in a certain complex analytic case. We emphasize that such uniqueness results are rare, and do not hold in classes of solutions to general elliptic or parabolic equations.

As a simple example of non-uniqueness for zero crossings of the heat equation, consider the case n=1, $A=\{(x,t)|x=0,t>0\}$. Clearly, any function f(x) which is odd about the origin, i.e., f(-x)=-f(x), will have A as a zero crossing. As long as 0 is the unique zero of f(x), A will be the sole zero crossing of the corresponding u(x,t). It is not nard to show, using Taylor series expansion of f(x) about x=0, that the only smooth functions yielding A as a zero crossing are odd functions.

As a second example which suggest more general non-uniqueness, consider a solution to the heat equation, u(x,t) with analytic initial data f(x), n = 1, having a single zero crossing curve which can be parameterized by

$$t = t(x), |x| \le a$$

where t(a) = t(-a) = 0, and t(x) > 0 elsewhere. We further suppose that the zero crossing curve contains no cusps, so that t(x) is analytic. We have that

$$u(x,t(x)) \equiv 0 \quad \text{for} \quad |x| \leq a. \tag{4.1}$$

Further, since u(x,t(x)) is an analytic function of x for |x| < a, a necessary and sufficient condition for (4.1) to hold is that all derivatives $\frac{d^n}{dx^n}$ (u(x,t(x)) vanish at x = a.

For simplicity, we assume that $t'(a) = \sigma$ with $0 < \sigma < \infty$. The cases $\sigma = 0$ and $\sigma = \infty$ can be treated similarly. Using the equations $u_t = u_{xx}$, and u(x,0) = f(x), we obtain from (4.1) by successive differentiations

$$u_x + u_{t^*}t'(x) = 0$$
,
 $u_{xx} + u_{tx^*}t' + u_{tt^*}(t')^2 = 0$,
etc.

Evaluating at x = a, we obtain constraints on f(x):

$$f'(a) + \sigma f''(a) = 0$$

 $f''(a) + \sigma f'''(a) + \sigma^2 f''''(a) = 0$

Thus f''(a) is determined from f'(a), and f''''(a) is determined from f'''(a) and f'(a). In general, by differentiating n times and evaluating at x = a, a linear constraint of the form

$$f^{(n)}(a) + ... + \sigma^n f^{(2n)}(a) = 0$$
 (4.2)

will be obtained. By induction we see that the even derivative $f^{(2n)}(a)$ is determined by the odd derivatives at a of order less than 2n.

Now, the system of equations (4.2) is also sufficient for an analytic function f(x) to give rise to a solution u(x,t) satisfying (4.1). Thus any analytic function satisfying (4.2) will have t = t(x) as a zero crossing curve. Since all odd derivatives of f(x) at x = a are free parameters in (4.2), it is reasonable to expect that there exists many such analytic functions f(x). Of course, most of these solutions will have other zero crossings. However, because of the large number of free parameters, perhaps perturbations of the original expansion for f(x) are possible which yield no new zero crossings.

We are currently conducting experiments to explore degeneracies in these and more complicated zero crossing surfaces situations.

Finally, we note how one might use the results from Section III to obtain multiple solutions to the inverse problem obtained by specifying the zero crossing surfaces of a solution to the heat equation. Ideally, one would like to augment the zero crossing data with

arbitrary gradient data, and then reconstruct using the algorithm of Section III. However, this procedure will in general fail to construct a solution with the same zero crossings as the original solution, and may even fail to yield data which can be backsolved to a function at t = 0. Instead, the gradient data must be constrained to satisfy an integral equation.

We illustrate the procedure and the integral condition by a simple example. Consider the case n=1 with a single smooth zero crossing surface Γ parameterized by x=x(t), t>0, starting at 0, x(0)=0 and extending to ∞ . The curve separates the (x,t) domain into two regions, D_1 on the left and D_2 on the right (see Figure 2).

We will determine a compatible pair of data

$$f(x) = u(x,0), x \le 0$$
 (4.3)

$$Q(t) = u_{X}(x(t), t), t > 0$$
 (4.4)

so that the solution to the heat equation defined by

$$u(x,t) = \int_{0}^{t} K(x-x(s), t-s)Q(s)ds$$

$$+ \int_{-\infty}^{0} K(x-y,t)f(y)dy, \qquad (4.5)$$

which automatically satisfies (4.3), will also vanish on Γ and satisfy (4.4).

The function f(x), $x \le 0$, should be chosen among smooth functions vanishing at 0 and $-\infty$, and nonzero elsewhere. However, f(x) cannot be

chosen arbitrarily. Instead, it must be chosen so that there exists a solution Q(t) to the Volterra-type integral equation

$$Q(t)/2 = \int_{0}^{t} K_{x}(x(t) - x(s), t-s)Q(s)ds$$

$$+ \int_{-\infty}^{0} K(x(t) - y,t)f'(y)dy \qquad (4.6)$$

In that case, we can show that u(x,t) defined in (4.5) has the required zero crossing Γ , and, incidentally, gradient data Q(t). Then by choosing different compatible pairs f(x), x < 0, and Q(t), different solutions u(x,t) can be obtained each giving Γ as a zero crossing surface. Of course, the ability to find one such pair depends on the curve Γ . Not all curves will be the zero crossing belonging to some initial data.

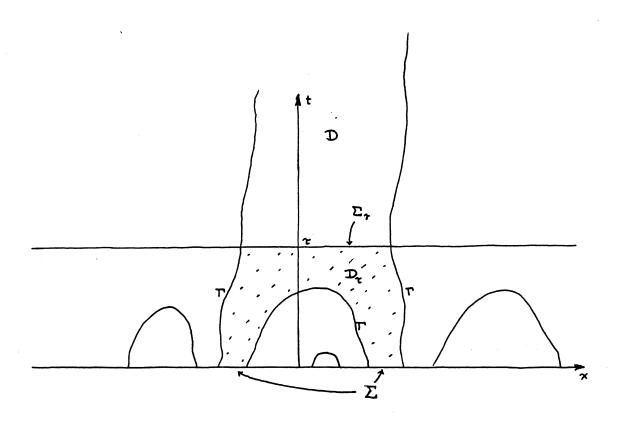


Figure 1. An unbounded component

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