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ANISOTROPIC RADIAL BASIS FUNCTIONS

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Abstract: There are multiple reasons why anisotropic basis functions may be needed or be more appropriate. The most obvious is that if the basis function is to be defined on $R^n \times T$ then there is no natural norm on this space that would reflect the unique properties of time. A second reason is that function being interpolated or approximated may incorporate a directional dependence. Thirdly, differentiability of the basis function is often critical, i.e., partial differentiability. Separating the differentiability from one dimension to another may be necessary, e.g., differentiability with respect to time as contrasted with differentiability with respect to a space coordinate. Positive definiteness (or conditional positive definiteness) is often dependent on the dimension of the space. Thus construction of non-radially symmetric basis functions which can easily be shown to be strictly positive definite is important, a number of examples and general methods will be given.

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1. The Importance of Positive Definiteness and Conditional Negative Definiteness

To ensure a unique solution for the coefficients in a radial basis function (RBF) interpolator or in the Kriging estimator it is necessary to have a positive definite function (p.d.), i.e., a covariance function or a conditionally negative definite function (c.n.d), i.e., a generalized covariance. In either case the function must be "strict", i.e., p.d. and not just non-negative definite [9], [1]. In geostatistics it is common to "fit" the data to a valid model

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(a covariance function or a variogram), see [5]. The software will normally provide the user with a list of valid isotropic (radial) models, positive linear combinations are also valid [6]. In the numerical analysis literature it is common to choose the basis function independently of the data.

2. Motivation for Anisotropic Basis Functions

Recall that $F(x)$ defined on R^d is radial (also called isotropic) if there is a function $f(x)$ defined on R such that $F(x) = f(||x||)$. Let B be an affine transformation on R^d, then $F^*(x) = f(||Bx||)$ is anisotropic (this is called a geometric anisotropy). There are at least two kinds of problems where an anisotropic basis function might be desirable. One is for the extension to space-time, i.e., the basis function is to be defined on $R^d \times T$. One might utilize a norm of the form $||h||^2 + c^2|t|^2$ but the resulting model has undesirable properties and does not scale well with changes in the units. A second instance is where the basis function is defined on $R^{d_1} \times R^{d_2}$ and the behavior of the function should be different on the two subspaces. Clearly the geometric anisotropy is not appropriate for either of these two cases, [8].

3. Some Important Properties and Connections

In general both positive definiteness and "strictness" are dimension dependent. For example the hat function is strictly p.d. on R but not on R^2. However both properties are inherited on lower dimensions.

3.1. Marginals

Let $C(x, y)$ be strictly p.d. on $R^{d_1} \times R^{d_2}$ then $C(x, 0)$ is strictly p.d. on R^{d_1} and $C(0, y)$ is strictly p.d. on R^{d_2}. Likewise if $\gamma(x, y)$ is strictly c.n.d. on $R^{d_1} \times R^{d_2}$ then $\gamma(x, 0)$ is strictly c.n.d. on R^{d_1} and $\gamma(0, y)$ is strictly c.n.d. on R^{d_2}. These associated functions are called *marginals*, see [2], [3]. These generalize to other decompositions of R^d and also of $R^d \times T$. Marginals may be projected on any lower dimensional space but it is likely that the most interesting ones are projected on 1-dimensional spaces.

3.2. Boundedness Properties

Positive definite functions (whether strict or not) are bounded but need not tend to zero at infinity. In the case of isotropic p.d. functions that have compact support or are asymptotic to zero, the distance a such $C(r) = 0$ for $r \geq a$ is called the range. In the case of p.d. functions with an geometric anisotropy the range may be directionally dependent. If the p.d. function is only asymptotic to zero then there still may be an "effective range", i.e., a distance such that $C(r) \leq .05C(0)$ for $r > a$. $C(0)$ is often called the "sill". In contrast c.n.d. functions need not be bounded but must grow at less than a quadratic rate. Recall that if $C(h)$ is p.d. on R^d, then

$$\gamma(h) = C(0) - C(h)$$

is c.n.d.. Conversely if a c.n.d function is asymptotically bounded then it can be written in this form.

3.3. Review of Algebraic Properties

If $C_1(x)$ is strictly p.d. on R^{d_1} and $C_2(y)$ is strictly p.d. on R^{d_2}, then $A_1C_1(x) + A_2C_2(y)$ is p.d. on $R^{d_1} \times R^{d_2}$ for any positive constants A_1, A_2 but not necessarily "strictly". However $C_1(x) \times C_2(y)$ is strictly p.d. on $R^{d_1} \times R^{d_2}$. Likewise, if $\gamma_1(x)$ is strictly c.n.d. on R^{d_1} and $\gamma_2(y)$ is strictly c.n.d. on R^{d_2}, then $A_1\gamma_1(x) + A_2\gamma_2(y)$ is c.n.d. on $R^{d_1} \times R^{d_2}$ for any positive constants A_1, A_2 but not necessarily "strictly". However in general $\gamma_1(x) \times \gamma(y)$ is not c.n.d., in particular it may not satisfy the quadratic growth rate.

4. Construction of Anisotropic Basis Functions

The level curves of isotropic basis functions are circles (or their analogues in higher dimensional spaces). Basis functions with a geometric anisotropy have elliptical level curves. More generally the level curves may be much more complex.

4.1. Product-Sum Model

Let $C_1(h), C_2(h')$ be strictly p.d. functions on R^{d_1}, R^{d_2} respectively and $A_1 > 0,\ A_2, A_3 \geq 0$, then

$$C(h,h') = A_1 C_1(h) \times C_2(h') + A_2 C_1(h) + A_3 C_2(h')$$

strictly p.d. on $R^{d_1} \times R^{d_2}$ If $\gamma(h,h')$ is the associated c.n.d. function then the product sum model may be written in the form

$$\gamma(h,h') = \gamma(h,0) + \gamma(0,h') - K\gamma(h,0) \times \gamma(0,h'),$$

where K is a constant satisfying $0 < K \leq (1/\max(C_1(0), C_2(0)))$, see [2], [3]. Hence given $\gamma_1(h), \gamma_2(h')$, asymptotically bounded strictly c.n.d. functions on R^{d_1}, R^{d_2} respectively then

$$\gamma(h,h') = \gamma_1(h) + \gamma_2(h') - K\gamma_1(h) \times \gamma_2(h')$$

is strictly c.n.d on $R^{d_1} \times R^{d_2}$. This will easily generalize to a product-sum involving more factors.

4.1.1. Powered Exponential Basis Function

For simplicity consider the case of R^3 then this basis function can be written in the form

$$C(x,y,z) = \exp(-(|x|/b_1)^{a_1} - (|y|/b_2)^{a_2} - (|z|/b_3)^{a_3}),$$

where $b_1, b_2, b_3 \geq 0$ and $0 < a_1, a_2, a_3 \leq 2$. This strictly p.d. function is the product of three strictly p.d. functione, each defined on a 1-dimensional subspace. The case of $a_1 = a_2 = a_3 = 1$ is just an exponential model that is widely used in hydrology. The case of $a_1 = a_2 = a_3 = 2$ is just a Gaussian model. To see how this generalizes, consider the case where $d_1 = d_2 = 1$ then the associated c.n.d. function is

$$\begin{aligned}\gamma(x,y) = 1 - \exp[-(|x|/b_1)^{a_1}] + 1 - \exp[-(|y|/b_2)^{a_2}]\\ - K12(1 - \exp[-(|x|/b_1)^{a_1}])\\ (1 - \exp[-(|y|/b_2)^{a_2}]) = (2 - K12) - (1 - K12)\exp[-(|x|/b_1)^{a_1}]\\ - (1 - K12)\exp[-(|y|/b_2)^{a_2}] - K12(\exp[-(|x|/b_1)^{a_1}])(\exp[-(|y|/b_2]^{a_2}).\end{aligned}$$

When $K12 = 1$ the model is just the powered exponential. Again this will easily generalized to more factors.

4.1.2. Truncated Linear-Hat Function

Let

$$C(x) = \begin{cases} 1 - |x|/b, & \text{if} \quad 0 \leq |x| \leq b, \\ 0, & \text{if} \quad |x| > b. \end{cases}$$

This is usually known as the hat function and is strictly p.d. on R but is not strictly p.d. on higher dimensional spaces, see [1]. The associated c.n.d function is sometimes known as the Truncated linear function. Either function can be extended to higher dimensions using a product-sum model. Let

$$\gamma_i(x) = \begin{cases} |x|/b_i, & \text{if} \quad 0 \leqq |x| \leq b_i, \\ 1, & \text{if} \quad |x| > b, \end{cases}$$

and set

$$\gamma(x, y) = \gamma_1(x) + \gamma(y) - K12\gamma_1(x)\gamma_2(y).$$

This function is strictly c.n.d on R^2. If $K12 = 1$ it reduces to the product model.

4.2. Some Comments on These Examples

a) The product-sum easily generalizes to more marginals, there will be additional constants in that case. The signs on these constants will alternate and the maximal value will decrease as the number of factors in the product increases.

b) In each of the product-sum generalizations above, each marginal was of the same type. This is not necessary, the generalization will reduce to the product with the maximal value of K12.

c) The component marginals in the product-sum models need not be isotropic (on the lower dimensional space).

4.3. The Extension to Space-Time

There are examples in the literature, where $R^d \times T$ is treated as a normed space, i.e. with a norm $||h|| + c^2|t|^2$, where the constant c^2 is supposed to compensate for the discrepancy between space and time. However this is not scale/unit change invariant. Thus the dependence on space and on time should be "separated", i.e. radially symmetric models on $R^d \times T$ would not be appropriate.

5. Gneiting's Construction for Space-time P.D. Functions

Beginning with Bochner's Theorem and properties of completely monotone functions, [4] essentially combined the two ideas.

As is well known, if $\phi(u)$ is a completely monotone function then $C(h) = \phi(||h||^2)$ is a radially symmetric (isotropic) p.d. function on R^d for all dimensions

Let $\phi(u), u > 0$ be a completely monotone function and $\psi(w), w > 0$ be any positive function with completely monotone derivative. W.l.o.g. assume that $\phi(0) = 1$ and $\psi(0) = 1$. Then

$$C(h,t) = [\sigma^2/\psi(|t|^2)^{d/2}]\phi(||h||^2/\psi(|t|^2))$$

is a strictly p.d. function on $R^d \times T$

Note the interaction between space and time, i.e., as the time increment increases the spatial dependence decreases. The spatial and temporal marginals are

$$C(h,0) = \sigma^2\psi(||h||^2)\,, \quad C(0,t) = [\sigma^2/\phi(|t|^2)^{d/2}]\,.$$

Using these marginals a product sum model can be constructed.

$$C_{ps}(h,t) = d_1[\sigma^4\phi(||h||^2)/\psi(|t|^2)^{d/2} + d_2\sigma^2\phi(||h||^2) + d_3[\sigma^2/\psi(|t|^2)^{d/2}]\,,$$

which still incorporates interaction but in a different way.

Geniting's construction might be used on $R^{d_1} \times R^{d_2}$ but there seems less justification for choosing one of the two subspaces play a special role in the interaction.

6. Problems and Summary

6.1. Theoretical

Because of the equivalence between p.d. functions and covariance functions it seems reasonable that for a spatial model, $C(h) = C(-h)$ (even for an anisotropic model). Likewise, it seems reasonable that for a space-time model, $C(h,t) = C(-h,t)$. However the following do not seem so reasonable: $C(h,t) = C(h,-t)$, $C(h,t) = C(-h,-t)$.

However both the product-sum models and Gneiting's model do satisfy these equalities.

6.2. Practical

Data is usually costly both in money and in time. If the data is collected by an instrument, once set up can it often collect data for many time points rather easily but each new setup will be costly. Hence data is often sparse in space but rich in time. This may lead to numerical problems, i.e., the coefficient matrix may be ill-conditioned.

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