

Research Notes

Nonparametric Estimation using SOS-Convexity

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1 Introduction

(YJ will write out this section summerizing our first-day discussion when he has time.)

2 SOS-Convex Regression

Given $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$, where $\mathbf{x}_i \in \mathbb{R}^p$ and $y_i \in \mathbb{R}$ for $i = 1, \dots, n$, recall that we have the equivalence between the following optimization problems:

$$\begin{aligned} & \text{minimize} && \sum_{i=1}^n (y_i - f(\mathbf{x}_i))^2 \\ & \text{s.t.} && f \text{ is convex.} \end{aligned} \tag{1}$$

$$\begin{aligned} & \text{minimize}_{\mathbf{z}, \boldsymbol{\beta}} && \sum_{i=1}^n (y_i - z_i)^2 \\ & \text{s.t.} && z_j \geq z_i + \boldsymbol{\beta}_i^T (\mathbf{x}_j - \mathbf{x}_i) \quad \forall i, j = 1, \dots, n. \end{aligned} \tag{2}$$

In particular, we can reduce the infinite-dimensional problem (1) into a finite-dimensional quadratic program (QP) (2), which can be efficiently solved. The solution to (2) can be viewed as a piecewise-linear convex function.

Here, we attempt to derive the analogous equivalence, i.e. find an equivalent convex optimization problem to the following optimization problem:

$$\begin{aligned} & \text{minimize} && \sum_{i=1}^n (y_i - f(\mathbf{x}_i))^2 \\ & \text{s.t.} && f \text{ is an SOS-convex polynomial of degree } 2d. \end{aligned} \tag{3}$$

Denote the vector of basis monomials up to degree k by $\mathbf{v}_k(\mathbf{x}) = (1, x_1, \dots, x_p, x_1^2, x_1 x_2, \dots, x_p^k)^T$, where $\mathbf{x} = (x_1, \dots, x_p)$. Then the length of $\mathbf{v}_k(\mathbf{x})$ is $\binom{k+p}{p}$. Let

$$A_k = \left\{ \boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_p) \in \mathbb{N}^p \left| \sum_{j=1}^p \alpha_j \leq k \right. \right\}.$$

Then, we may represent f by a coefficient vector $\boldsymbol{\theta} \in \mathbb{R}^s$ ($s = \binom{2d+p}{p}$), such that

$$f(\mathbf{x}) = \boldsymbol{\theta}^T \mathbf{v}_{2d}(\mathbf{x}) = \sum_{\boldsymbol{\alpha} \in A_{2d}} \theta_{\boldsymbol{\alpha}} \mathbf{x}^{\boldsymbol{\alpha}},$$

where $\mathbf{x}^{\boldsymbol{\alpha}} = x_1^{\alpha_1} \dots x_p^{\alpha_p}$. Note the one-to-one correspondence between f and $\boldsymbol{\theta}$.

Further, as done with the convex program, we introduce the auxiliary variable $\mathbf{z} = (z_1, \dots, z_n)$ so that

$$f(\mathbf{x}_i) = \boldsymbol{\theta}^T \mathbf{v}_{2d}(\mathbf{x}_i) = z_i \quad \forall i = 1, \dots, n. \tag{4}$$

We can write this more concisely by introducing the matrix

$$V = V(\mathbf{x}_1, \dots, \mathbf{x}_n) = \begin{bmatrix} \mathbf{v}_{2d}(\mathbf{x}_1)^T \\ \vdots \\ \mathbf{v}_{2d}(\mathbf{x}_n)^T \end{bmatrix}_{n \times s}$$

so that (4) simply becomes

$$V\boldsymbol{\theta} = \mathbf{z}. \quad (5)$$

So we have a linear constraint on the coefficient $\boldsymbol{\theta}$ that is equivalent to saying that the polynomial interpolates the points $\{(\mathbf{x}_i, z_i)\}_{i=1}^n$. Analogously, we can rewrite the objective to be

$$\sum_{i=1}^n (y_i - z_i)^2 = \|\mathbf{y} - \mathbf{z}\|^2 \quad (6)$$

where $\mathbf{y} = (y_1, \dots, y_n)$ and $\mathbf{z} = (z_1, \dots, z_n)$.

Now we want to rewrite the constraint that $f(\mathbf{x}) = \boldsymbol{\theta}^T \mathbf{v}_{2d}(\mathbf{x})$ is SOS-convex. Recall that f is SOS-convex if and only if the polynomial $\mathbf{u}^T H_{\boldsymbol{\theta}}(\mathbf{x}) \mathbf{u}$ is sos in $(\mathbf{x}, \mathbf{u}) \in \mathbb{R}^{2p}$, where $H_{\boldsymbol{\theta}}(\mathbf{x})$ is the Hessian of f .

For $i, j \in \{1, \dots, p\}$ we have

$$H_{\boldsymbol{\theta}}(\mathbf{x})_{ij} = \frac{\partial^2 f(\mathbf{x})}{\partial x_i \partial x_j} = \sum_{\boldsymbol{\alpha} \in A_{2d}} \theta_{\boldsymbol{\alpha}} \frac{\partial^2 \mathbf{x}^{\boldsymbol{\alpha}}}{\partial x_i \partial x_j} = \begin{cases} \sum_{\boldsymbol{\alpha} \in A_{2d}} \theta_{\boldsymbol{\alpha}} \alpha_i \alpha_j \mathbf{x}^{\boldsymbol{\beta}_{\boldsymbol{\alpha}, i, j}} & (i \neq j) \\ \sum_{\boldsymbol{\alpha} \in A_{2d}} \theta_{\boldsymbol{\alpha}} \alpha_i (\alpha_i - 1) \mathbf{x}^{\boldsymbol{\beta}_{\boldsymbol{\alpha}, i, i}} & (i = j) \end{cases} = \sum_{\boldsymbol{\alpha} \in A_{2d}} c_{\boldsymbol{\alpha}, i, j} \theta_{\boldsymbol{\alpha}} \mathbf{x}^{\boldsymbol{\beta}_{\boldsymbol{\alpha}, i, j}} \quad (7)$$

where

$$\boldsymbol{\beta}_{\boldsymbol{\alpha}, i, j} = \begin{cases} (\alpha_1, \dots, \max(\alpha_i - 1, 0), \dots, \max(\alpha_j - 1, 0), \dots, \alpha_p) & i \neq j \\ (\alpha_1, \dots, \max(\alpha_i - 2, 0), \dots, \alpha_p) & i = j \end{cases}$$

and

$$c_{\boldsymbol{\alpha}, i, j} = \begin{cases} \alpha_i \alpha_j & i \neq j \\ \alpha_i (\alpha_i - 1) & i = j. \end{cases}$$

Then we have

$$\mathbf{u}^T H_{\boldsymbol{\theta}}(\mathbf{x}) \mathbf{u} = \sum_{i, j=1}^p \left(\sum_{\boldsymbol{\alpha} \in A_{2d}} c_{\boldsymbol{\alpha}, i, j} \theta_{\boldsymbol{\alpha}} \mathbf{x}^{\boldsymbol{\beta}_{\boldsymbol{\alpha}, i, j}} \right) u_i u_j,$$

which can be further written as

$$\mathbf{u}^T H_{\boldsymbol{\theta}}(\mathbf{x}) \mathbf{u} = \sum_{1 \leq i \leq j \leq p} \sum_{\boldsymbol{\beta} \in A_{2d-2}} h_{\boldsymbol{\theta}}(\boldsymbol{\beta}, i, j) \mathbf{x}^{\boldsymbol{\beta}} u_i u_j \quad (8)$$

where

$$h_{\boldsymbol{\theta}}(\boldsymbol{\beta}, i, j) = \begin{cases} (\beta_i + 2)(\beta_i + 1) \theta_{(\beta_1, \dots, \beta_i + 2, \dots, \beta_p)} & i = j \\ 2(\beta_i + 1)(\beta_j + 1) \theta_{(\beta_1, \dots, \beta_i + 1, \dots, \beta_j + 1, \dots, \beta_p)} & i < j. \end{cases}$$

It is then easy to see that $\mathbf{u}^T H_{\boldsymbol{\theta}}(\mathbf{x}) \mathbf{u}$ is SOS if and only if

$$\mathbf{u}^T H_{\boldsymbol{\theta}}(\mathbf{x}) \mathbf{u} = \mathbf{v}'_d(\mathbf{x}, \mathbf{u})^T Q \mathbf{v}'_d(\mathbf{x}, \mathbf{u}) \quad (9)$$

$$Q \succeq 0 \quad (10)$$

where $\mathbf{v}'_d(\mathbf{x}, \mathbf{u})$ is the vector of all monomials in (\mathbf{x}, \mathbf{u}) in which the degrees of all x_i 's have sum at most $d-1$ and there is exactly one u_i , i.e.,

$$\mathbf{v}'_d(\mathbf{x}, \mathbf{u}) = (u_1 \mathbf{v}_{d-1}(\mathbf{x})^T, u_2 \mathbf{v}_{d-1}(\mathbf{x})^T, \dots, u_p \mathbf{v}_{d-1}(\mathbf{x})^T)^T.$$

The length of $\mathbf{v}'_d(\mathbf{x}, \mathbf{u})$ is $r = p \binom{p+d-1}{p}$. Q is a $r \times r$ matrix.

(9) is not a valid semidefinite constraint yet, because it is an equality between two polynomials. This means we want to equate the *coefficients* of the two polynomials on (\mathbf{x}, \mathbf{u}) . The left-hand side is given by (8). Further, we can express the right-hand side in terms of their coordinates in the following way. First define the coordinate matrix $B_{\beta, i, j}$ for each $\beta \in A_{2d-2}, 1 \leq i \leq j \leq p$ such that

$$\mathbf{v}'_d(\mathbf{x}, \mathbf{u}) \mathbf{v}'_d(\mathbf{x}, \mathbf{u})^T = \sum_{1 \leq i \leq j \leq p} \sum_{\beta \in A_{2d-2}} B_{\beta, i, j} \mathbf{x}^\beta u_i u_j.$$

Note that the matrices $B_{\beta, i, j}$'s are simply "constants", i.e. they only depend on d (and p). With this, the right-hand side of (9) becomes

$$\begin{aligned} \mathbf{v}'_d(\mathbf{x}, \mathbf{u})^T Q \mathbf{v}'_d(\mathbf{x}, \mathbf{u}) &= \text{tr}(Q \mathbf{v}'_d(\mathbf{x}, \mathbf{u}) \mathbf{v}'_d(\mathbf{x}, \mathbf{u})^T) \\ &= \langle Q, \mathbf{v}'_d(\mathbf{x}, \mathbf{u}) \mathbf{v}'_d(\mathbf{x}, \mathbf{u})^T \rangle \\ &= \left\langle Q, \sum_{1 \leq i \leq j \leq p} \sum_{\beta \in A_{2d-2}} B_{\beta, i, j} \mathbf{x}^\beta u_i u_j \right\rangle \\ &= \sum_{1 \leq i \leq j \leq p} \sum_{\beta \in A_{2d-2}} \langle Q, B_{\beta, i, j} \rangle \mathbf{x}^\beta u_i u_j \end{aligned} \quad (11)$$

where $\langle A, B \rangle = \text{tr}(A^T B) = \sum_{i, j} A_{ij} B_{ij}$ is the matrix inner product. Note that Q is symmetric.

Then, we can equate the coefficients of (8) and (11) to obtain:

$$\langle Q, B_{\beta, i, j} \rangle = h_{\theta}(\beta, i, j) \quad \forall \beta \in A_{2d-2}, 1 \leq i \leq j \leq p \quad (12)$$

Putting (5), (6), (10), and (12) together, (3) can be restated as the following problem:

$$\begin{aligned} \underset{\mathbf{z}, \theta, Q}{\text{minimize}} \quad & \|\mathbf{y} - \mathbf{z}\|^2 \\ \text{s.t.} \quad & V\theta = \mathbf{z} \\ & \langle Q, B_{\beta, i, j} \rangle = h_{\theta}(\beta, i, j) \quad \forall \beta \in A_{2d-2}, 1 \leq i \leq j \leq p \\ & Q \succeq 0 \end{aligned} \quad (13)$$

(13) is almost an SDP, except that the objective is quadratic. But in general, we can introduce another auxiliary variable t to restate the problem as

$$\begin{aligned} \underset{t, \mathbf{z}, \theta, Q}{\text{minimize}} \quad & t \\ \text{s.t.} \quad & \|\mathbf{y} - \mathbf{z}\|^2 \leq t \\ & V\theta = \mathbf{z} \\ & \langle Q, B_{\beta, i, j} \rangle = h_{\theta}(\beta, i, j) \quad \forall \beta \in A_{2d-2}, 1 \leq i \leq j \leq p \\ & Q \succeq 0 \end{aligned} \quad (14)$$

Then, we are left with a quadratic inequality constraint. Fortunately, the following allows us to convert this into a semidefinite constraint.

Lemma 2.1 *For any $\mathbf{x}, \mathbf{q} \in \mathbb{R}^p$ and $r \in \mathbb{R}$, $\mathbf{x}^T \mathbf{x} + \mathbf{q}^T \mathbf{x} + r \leq 0$ if and only if $\begin{bmatrix} I & -\mathbf{x} \\ -\mathbf{x}^T & -\mathbf{q}^T \mathbf{x} - r \end{bmatrix} \succeq 0$.*

Proof: For any $\mathbf{y} \in \mathbb{R}^p$ and $z \in \mathbb{R}$,

$$\begin{aligned} \begin{bmatrix} \mathbf{y}^T & z \end{bmatrix} \begin{bmatrix} I & -\mathbf{x} \\ -\mathbf{x}^T & -\mathbf{q}^T \mathbf{x} - r \end{bmatrix} \begin{bmatrix} \mathbf{y} \\ z \end{bmatrix} &= \mathbf{y}^T \mathbf{y} - 2z \mathbf{x}^T \mathbf{y} - z^2 (\mathbf{q}^T \mathbf{x} + r) \\ &= \|\mathbf{y} - z \mathbf{x}\|^2 - z^2 (\mathbf{x}^T \mathbf{x} + \mathbf{q}^T \mathbf{x} + r). \end{aligned}$$

If $\mathbf{x}^T \mathbf{x} + \mathbf{q}^T \mathbf{x} + r \leq 0$, then this is nonnegative for all $\mathbf{y} \in \mathbb{R}^p$ and $z \in \mathbb{R}$. Otherwise, one can find $\mathbf{y} \in \mathbb{R}^p$ and $z \in \mathbb{R}$ such that this is strictly negative. ■

Thus,

$$\begin{aligned} \|\mathbf{y} - \mathbf{z}\|^2 \leq t &\iff \mathbf{z}^T \mathbf{z} - 2\mathbf{y}^T \mathbf{z} + (\mathbf{y}^T \mathbf{y} - t) \leq 0 \\ &\iff \begin{bmatrix} I & -\mathbf{z} \\ -\mathbf{z}^T & 2\mathbf{y}^T \mathbf{z} - \mathbf{y}^T \mathbf{y} + t \end{bmatrix} \succeq 0. \end{aligned}$$

Note that the last relation is a linear matrix inequality (LMI), i.e. it says that a linear combination of symmetric matrices is positive semidefinite.

Thus, we can now write (14) into a semidefinite program:

$$\begin{aligned} &\underset{t, \mathbf{z}, \boldsymbol{\theta}, Q}{\text{minimize}} && t \\ &\text{s.t.} && \begin{bmatrix} I & -\mathbf{z} \\ -\mathbf{z}^T & 2\mathbf{y}^T \mathbf{z} - \mathbf{y}^T \mathbf{y} + t \end{bmatrix} \succeq 0 \\ &&& V\boldsymbol{\theta} = \mathbf{z} \\ &&& \langle Q, B_{\boldsymbol{\beta}, i, j} \rangle = h_{\boldsymbol{\theta}}(\boldsymbol{\beta}, i, j) \quad \forall \boldsymbol{\beta} \in A_{2d-2}, 1 \leq i \leq j \leq p \\ &&& Q \succeq 0 \end{aligned} \tag{15}$$

where the two semidefinite constraints can be restated – if necessary – into one semidefinite constraint

$$\begin{bmatrix} I & -\mathbf{z} \\ -\mathbf{z}^T & 2\mathbf{y}^T \mathbf{z} - \mathbf{y}^T \mathbf{y} + t \\ & & Q \end{bmatrix} \succeq 0.$$

Finally, note that the entire program depends on the degree of the SOS-convex polynomial that we started off with: $2d$.

Further Questions

1. What is the program size? Is it tractable?
2. For any given d , is the program feasible? What is the behavior of the objective t_d ?
3. How can SDP hierarchy (e.g. by Lasserre) help choosing/removing d ?

3 Convexity Pattern Problem

We now consider a more restricted family of distributions that are hopefully more tractable and also have interesting applications.

With the familiar regression setting as in (1), first consider the additional constraint that f is not only convex but also a function of only a few variables from $\mathbf{x} = (x_1, \dots, x_p)$. For example, we may have

$$f(x_1, \dots, x_p) = f(x_1, x_2) \quad \forall \mathbf{x} \in \mathbb{R}^p$$

as one of the possibilities.

In [DCM], Qi, Xu, and Lafferty shows a way to approximate the solution to the above problem *additively*. Specifically, this is

$$\begin{aligned} & \underset{f_1, \dots, f_p}{\text{minimize}} && \sum_{i=1}^n (y_i - \sum_{j=1}^p f_j(x_{ij}))^2 \\ & \text{s.t.} && f_1, \dots, f_p \text{ convex} \end{aligned} \tag{16}$$

where $\mathbf{x}_i = (x_{i1}, \dots, x_{ip}) \in \mathbb{R}^p$. In other words, we have the model

$$Y = \sum_{j=1}^p f_j(X_j) + \varepsilon$$

in the population, with random variables $X = (X_1, \dots, X_p) \in \mathbb{R}^p$ and $Y \in \mathbb{R}$.

We can view this as a problem of *sparsity patterns*, i.e. whether each variable is “relevant” ($f_j \not\equiv 0$) or not ($f_j \equiv 0$), and it is clear that there are 2^p sparsity patterns with p variables.

Here, we consider an analogous problem of choosing whether each f_j is convex or concave. Naturally, there are 2^p *convexity patterns*. We can write this problem as the following optimization problem:

$$\begin{aligned} & \underset{\mathbf{Z}, \mathbf{f}, \mathbf{g}}{\text{minimize}} && \sum_{i=1}^n \left(y_i - \sum_{j=1}^p [Z_j f_j(x_{ij}) + (1 - Z_j) g_j(x_{ij})] \right)^2 \\ & \text{s.t.} && Z_1, \dots, Z_p \in \{0, 1\} \\ & && f_1, \dots, f_p \text{ convex} \\ & && g_1, \dots, g_p \text{ concave} \end{aligned} \tag{17}$$

Note that Z_1, \dots, Z_p are 0/1-boolean variables and $f_1, \dots, f_p, g_1, \dots, g_p$ are univariate functions.

In order to make the problem more tractable, we first give extra constraints: namely, that $f_1, \dots, f_p, g_1, \dots, g_p$ are *polynomials*. It is important to note that a univariate polynomial is convex if and only if it is SOS-convex. [Problem: Is the set of convex polynomials dense in the set of convex functions? Is

this relevant?] We can rewrite the program as follows:

$$\begin{aligned}
& \underset{\mathbf{Z}, \mathbf{f}, \mathbf{g}}{\text{minimize}} && \sum_{i=1}^n \left(y_i - \sum_{j=1}^p [Z_j f_j(x_{ij}) + (1 - Z_j) g_j(x_{ij})] \right)^2 \\
& \text{s.t.} && Z_1, \dots, Z_p \in \{0, 1\} \\
& && f_1, \dots, f_p \text{ are (SOS-)convex polynomials of degree at most } d \\
& && g_1, \dots, g_p \text{ are (SOS-)concave polynomials of degree at most } d
\end{aligned} \tag{18}$$

Using the similar trick as above, we hope to convert the constraints on $f_1, \dots, f_p, g_1, \dots, g_p$ into linear or semidefinite ones.

A more important feature of this program is the use of 0-1 variables. It is well-known that, in general, solving a 0-1 integer linear program is NP-hard, and one of the standard procedures in theoretical computer science in dealing with this problem is to relax it such that the boolean constraint is replaced by $Z_1, \dots, Z_p \in [0, 1]$, or equivalently the quadratic constraint $Z_j^2 - Z_j \leq 0 \ \forall j = 1, \dots, p$.

With this relaxation comes a family of LP/SDP hierarchies, such as the ones developed by Lovász-Schrijver, Sherali-Adams, and Lasserre. [Prof. Madhur Tulsiani's Survey] These hierarchies are all a sequence of convex programs (LPs or SDPs) whose objective approaches the actual 0-1 solution.

A good way to think about the hierarchies for 0-1 programs is to consider the Z_j 's the marginals of a distribution over a set of 0-1 solutions. Specifically, in the initial "round", consider Z_j to be the marginal of the solution whose j th entry is 1 and all others are zero. Then, in consecutive rounds, the goal is to add the *joint probabilities* between these variables – in the r th round, we consider the joint random variables Z_S for each $S \subseteq \{1, \dots, p\}$ such that $|S| \leq r$. One can think of these "big variables" as $Z_S = \mathbb{E} \left[\prod_{j \in S} Z_j \right]$, i.e. the probability that all variables in S are 1.

Our hope is to use one of the hierarchies to solve a set of relaxations of (18) that approximates the actual solution efficiently.

4 Log-SOS-Concave Density Estimation

References

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