

## Peer Review File

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### Reviewer A

We would like to congratulate the authors on their manuscript entitled: prediction of postoperative final degree and recurrence of pectus excavatum using machine learning algorithms. Please find our comments below.

Comment 1: General comment:

- Does the word limit of the abstract adhere to the JTD guidelines?

Response 1: Yes. The word limit of the abstract is 200–350 words. Our number of words in the abstract is 349 words.

Comment 2: Introduction: - Accepted practice is to remain the bar in situ for 3 years.

Response 2: Our practice is different according to age of patients. Duration of bar placement is about two years for the early repair and three years for the late repair, which is widely accepted in Korea (J Thorac Cardiovasc Surg 2010 Feb;139(2):379-86).

Comment 3: What is meant by final degree in line 82?

Response 3: This is the final degree of pectus excavatum, which is presented by RPI. We wrote “.... predict final degree and recurrence of PE.....”

Comment 4-Materials and methods: What is the rationale for the lower bound of the enrollment period being March 2012? Was this the date of the first surgery ever performed at Uijeongbu Saint Mary’s hospital?

Response 4: Yes. The date is my first surgery at Uijeongbu Saint Mary’s hospital.

Comment 5- Would it be possible to include data on patients from 2020-2023? It feels as if aged data is being presented.

Response 5: Of course, I can include data on patients from 2020-2023. However, there was a major change of the operation technique from 2020 and we have adopted the bridge technique for pectus bar fixation (J Pediatr Surg 2015 Aug;50(8):1320-2). To reduce the heterogeneity of data, I think that it had better exclude data from 2020-2023. Because this new technique can reduce pectus bar displacement, I assume that prediction can be more accurate when this data is used. I will study this topic using this data.

Comment 6- What is the rationale to obtain two-view x-rays daily?

Response 6: Initially, we obtained two-view x-rays for early and accurate detection of bar displacement (shift and rotation) and complications. However, we found that two-view x-rays provide quantified data of the bar displacement, and a radiographical postoperative degree of pectus excavatum without chest CT scans. Therefore, we routinely obtain two-view x-rays daily.

Comment 7- It is said that CT scans were routinely acquired but then also that a complete series of chest CT scans was not available to calculate the HI from? Please explain.

Response 7: I think that we should not obtain CT scans only for HI. We obtain CT scans only perioperative periods (before and after bar insertion and removal). Because chest CT scan is not obtained on an outpatient basis during follow-ups, we do not know HI using chest CT scan. I revised the manuscript to clarify the meanings as your comments.... because a complete series of chest CT scans for the Haller index was not available an outpatient basis during follow-ups....

Comments 8- The lengths were calculated in double-blind fashion. That means that two measurements are at least available. What value is chosen for the final analysis?

Response 8: The measurement was performed by authors. In our study, double-blind fashion means that one measured posteroanterior lengths and other measured transverse lengths. In addition. The data were randomly distributed to authors.

Comment 9- How was the cut-off for re-depression chosen? Arbitrarily?

Response 9: Thanks for your comments. Re-depression is defined when cases met both conditions: increased RPI value and RPI value  $\geq 3.5$  after BR. As your comments, the cut-off value of RPI 3.5 is arbitrarily but this value is mean RPI value of immediate value after bar removal in recurrent group. We need further studies on the definition of re-depression of chest wall.

Comment 10- In addition, how do these values translate to the clinical picture? Are these clinically relevant? A slight increase in RPI may not be clinically significant.

Response 10: Thanks for your raising an important issue. Final degree of chest wall depression generally improved even in re-chest wall depression cases. Therefore, we ignore mild re-depression after completion of treatment. However, we effort to minimize the re-depression for patient's satisfaction and to reduce re-operation cases.

Comment 11- Moreover, during the Nuss procedure one tends to overcorrect the deformity by approximately 10% which can depress after bar removal. Is this considered re-depression?

Response 11: Thanks for your comments. Re-depression is defined when cases met both conditions: increased RPI value and RPI value  $\geq 3.5$  after BR. If re-depression of 10% developed, RPI value  $< 3.5$  is not defined as recurrence.

Comment:12- What is the difference between RPI and HI? In my opinion none.

Response 12: Both indicate the degree of pectus excavatum. The standard degree is HI from chest CT scan. RPI has an advantage that can be obtained simply from simple chest x-rays. However, measuring degree of chest wall depression by simple radiography could result in measurement errors that could be influenced by physiologic factors, especially in the asymmetric type. These were commented in limitations section of this study.

Comment 13- What was the rationale to divide patients with a cut-off of 10 years?

Response 13: This is also somewhat arbitrary, but we empirically divided patients by age of ten (early vs. late repair). I published the paper titled as A cross-sectional study for the development of growth of patients with pectus excavatum (Eur J Cardiothorac Surg. 2016 Dec;50(6):1102-1109). This study showed that development of growth in patients with pectus excavatum is retarded and appears to be related to the severity of pectus excavatum. The development of growth can be recovered by early correction of the deformity. In addition, I published the paper titled as Recurrence of pectus excavatum following the Nuss procedure (J Thorac Dis . 2018 Nov;10(11):6201-6210.). This study showed that the effect of MIRPE is different according to the patient age at the time of the procedure. Early correction of PE can provide better corrective results because of the existence of a more pliable chest wall, which can be easily and sufficiently elevated by the MIRPE. Early correction means a repair before age of ten.

Comment 14: - Why where statistical analysis performed between groups according to age? This isn't the rationale for this study? The analysis used and the groups defined should answer the research question at the end of your introduction.

Reponses 14: We mentioned in introduction section that the primary aims of the present study are to investigate characteristics of chest wall re-depression and to predict final degree and recurrence of PE after BR using machine learning algorithms. The age is an important factor for re-depression of chest wall after bar removal. In addition, we mentioned in methods and material section that "Third, to determine the optimal age at the time of MIRPE, we divided the subjects into two groups by age ( $< 10$  years (early repair group; EG) vs.  $\geq 10$  years (late repair group; LG)) when they underwent MIRPE and examined the relationship between age and recurrence".

Comment 15: Results/discussion - There is quite a big difference of the mean duration of bar placement between both groups. Please explain.

Reply 15: In our practice, bar placement is generally maintained for two to three years according to patient conditions, especially such as ages. Bar placement is maintained for about two years in pediatric patients, for about three years for elderly patients.

Comment 16:- Why compare the HI and RPI? This has been performed extensively as well been validated in prior studies.

Reponses 16: Indeed, prior studies have shown validity of RPI. However, RPI is not officially accepted. In addition, this term is not well known.

Comment 17:- Line 184 is part of the discussion. In addition, the ideal age is >12years.

Response 17: Thanks for your comments. There are debates regarding recurrence after BR and the ideal age for MIRPE. We assumed that early correction before age of ten is better than late one. I think that diverse opinions and researches are valuable in uncovering the truth.

Comments 18: - How should we use these algorithms in daily clinic?

Response 18: We used The Orange® data mining toolbox. The Orange® data mining toolbox in Python (Bioinformatics Lab at University of Ljubljana, Slovenia) was used for machine learning models learning (16). This open-source platform is a machine learning and data mining suite for data analysis through Python scripting and visual programming. the strongest is that we can easily use algorithms without coding.

Comment 19- The haller index/RPI are known to be a bad descriptor of the 3-dimensional structure of the pectus excavatum; how should we interpret these results?

Response 20: Thanks for your comments. I undoubtedly agree with your comments. PE cannot be simply and strictly defined into two types (symmetric vs. asymmetric) because it has many variant morphologies. In addition, RPI cannot describe the complete degree of PE. The heterogeneity in PE type and incomplete descriptions of degree reflect real-world situations, and machine learning models trained with such data may be more appropriate for clinical practice. Further, I hope the 3D analysis with more advanced artificial intelligence tools. These are commented in the limitations section.

#### **Reviewer B**

The authors present a retrospective study including 199 pectus excavatum (PE) patients who underwent minimally invasive repair of PE (MIRPE) and subsequently pectus bar removal (BR), after 28.5 months on average. Chest x-ray in 2 planes were acquired every day during hospitalization and at every outpatient follow-up appointment, and additionally thoracic CT scan were done before and on 3rd postoperative day after both MIRPE and BR. PE patients were divided into early group ( < 10y). Machine learning algorithms considering risk factors were applied to predict chest wall re-depression after BR.

Even if the idea and concept of the current study is very interesting, the manuscript has to be considered as not appropriate for publication in the JTD in the current version.

The reviewer has some basic concerns about clinical practice and study design (which would not be accepted by the local ethics committee):

Comments 1: indication for MIRPE in patients under the age of 10 years? Please clarify (symptoms?)

Response 1: Thanks for your raising a basic issue. I think that there is no limitation on age at the surgery and early repair is better than late one, which is suggested by many prior papers (Eur J Cardiothorac Surg . 2012 Oct;42(4):667-72, etc) and my preference. The rationales for early repair are developmental benefit, lower risk for complications, easier repair, and lower recurrence, etc. In addition, symptoms of pectus excavatum are rarely observed and indication for surgery usually depends on morphological degree of pectus excavatum.

Comment 2: chest x-ray pa and lateral on every day during hospitalization? What is the indication for a such a high radiation exposure?

Response 2: Thanks for your comments. I am afraid of a possible high radiation exposure, but hospitalization is only a few days. I am sure that chest x-ray pa and lateral views provide early detection of complications, such as bar migration, which ensure patient safety and good postoperative outcomes.

Comment 3- thoracic ct scan after MIRPE and BR, again please clarify the indication for radiation exposure.

Response 4: I agree with your concerns. We routinely performed chest CT scans without enhancement, which reduces radiation exposure. We obtain chest CT four times for 2-3 years, which is considered

acceptable for treatment. Chest CT scans enable early detection of complications and better outcomes after surgery.

Comment 5- Haller index as well as radiographic pectus index may be obtained by chest x-ray

Response 5: I agree that both index indicates degree of pectus excavatum. However, Haller index is calculated using chest CT and radiographic pectus index is calculated using simple chest x-rays. In addition, measuring degree of chest wall depression by simple radiography could result in measurement errors that could be influenced by physiologic factors, especially in the asymmetric type.

Comment 6: - BR after 28.5 months on average; majority of pectus surgeons including Dr. Nuss and his team recommend BR after 36 months; please commend

Response 6: Thanks for your comments. I agree with an issue on duration of bar placement. Our practice is different according to age of patients. Duration of bar placement is two years for early repair and about three years for late repair, which is widely accepted in Korea (J Thorac Cardiovasc Surg 2010 Feb;139(2):379-86)

Comment 7- number of pectus bars (table 1): 128 = 1 bar; 71 = more than 2 bars?? please clarify

Response 7: Two bars 69 cases and three bars two cases were found. I revised the table as your comments.

Comment 8- statement "chest wall re-depression generally deteriorates only for the first 6 months after BR" - please clarify and confirm; many pectus surgeons have different experience and follow-up their patients at least 12-18 months after BR.

Reponses 8: Thanks for your raising an important issue. This study showed that the patterns of chest wall re-depression after bar removal are different according to recurrence. RPI of the recurrent group continuously increased after BR during observation periods while RPI of the non- recurrent group did not increase after six months following BR. I think that this issue should be validated by further long-term studies.

Comment 9- statement "2nd problem is the defining recurrence of PE"; the reviewer agrees that is correct/a problem; what is about the clinical aspect? As mentioned in the "limitation" section, the definition of recurrence will affect the results, and has to be defined.

Response 9: I agree with your concerns. Final degree of chest wall depression generally improved even in re-chest wall depression cases. Therefore, we ignore mild re-depression after completion of treatment. However, we effort to minimize the re-depression for patient's satisfaction and to reduce re-operation cases. Recurrence is defined when cases met both conditions: increased RPI value and RPI value  $\geq 3.5$  after BR in this study, which is documented in the Materials and Methods section. Indeed, we need consensus on the definition of recurrence.

Comment 10- statement "we conclude that early repair of PE is better than late repair with respect to recurrence" - this statement is in contrast to the results of many studies including larger number of patients (with - by the way - lower recurrence rates)

Response 10: Thanks for your raising an important issue. In the present study, we found that the recurrence rate was lower in the early repair group than in the late repair group, although the change of RPI after BR showed similar patterns between groups. The lower rate of recurrence in the early repair group was explained by RPI values before and after MIRPE and age group, which were identified as independent risk factors of recurrence after BR. RPI values before and after MIRPE was lower in the early repair group than in the late repair group, although the degree and pattern of chest wall re-depression after bar remove did not differ by age. These findings are explained by the reliance of MIRPE on chest wall pliability, which may weaken with age. We conclude that early repair better than late repair with respect to recurrence, and the corrective effect of MIRPE was higher in the early than in the late repair. I published this suggestions (A cross-sectional study for the development of growth of patients with pectus excavatum (Eur J Cardiothorac Surg. 2016 Dec;50(6):1102-1109: Recurrence of pectus excavatum following the Nuss procedure (J Thorac Dis . 2018 Nov;10(11):6201-6210).

Comment 11: worsening of pectus deformity during puberty growth spurt - could you differentiate between a "real" recurrence and the effect of pubertal growth?

Response 11: Thanks for your important comments. To the best of my knowledge, developmental study on

the association between puberty growth spurt and pectus excavatum is insufficiently investigated. However, we empirically recognize deterioration of pectus excavatum during puberty growth spurt. I think that pectus excavatum had better be repaired before this deterioration during puberty. Perfect repair can prevent recurrence during puberty.

### Reviewer C

The prediction of postoperative degree and recurrence of pectus excavatum is undoubtedly an important, albeit insufficiently investigated, clinical topic. Your work provides valuable insights into complex pathology and surgical procedures. Nonetheless, there are some areas that could be refined to further augment the quality and impact of your manuscript. Here are some respectful suggestions and questions that could potentially improve your paper if you choose to implement them:

Abstract:

Comment 1: Abstract:- The abstract clearly summarizes the key aspects of the study. To make it more impactful for readers, consider highlighting the novelty and significance of using machine learning algorithms in the prediction of surgical outcomes following MIRPE.

Response 1: Thanks for your comments. We revised the manuscript to highlight the novelty and significance as your comments. I revised the background section in the abstract as “Chest wall re-depression after bar removal (BR) in pectus excavatum is insufficiently investigated. However, it is not easy to investigate chest wall re-depression due to its multifactorial characteristics. Herein, we investigated chest wall re-depression after BR using machine learning algorithms. To the best of my knowledge, this is the first study of chest wall re-depression after BR using machine learning algorithms”.

Comment 2: Introduction-The introduction provides good background on the clinical issues regarding recurrence after MIRPE. You may consider emphasizing why developing predictive models is an important goal for improving management of patients undergoing this type of surgery.

Responses 2: Thank for your comments. I revised the manuscript as your comments. I added the sentences “The prediction models using machine learning for chest wall re-depression after BR are valuable for better surgical outcomes because machine learning has successfully been used to make accurate decisions and predictions using diverse and large amounts of data.”

Comment 3- Providing more background on prior attempts or limitations in predicting surgical outcomes for pectus excavatum would better contextualize the rationale for a machine learning approach.

Responses 3: Thank for your comments. I revised the manuscript as your comments. I added this sentence “However, prior studies are insufficient in prediction of surgical outcomes in PE”.

Comment 4: Methods: - Considering the potential limited adoption of the RPI by surgeons, it could be beneficial to include additional information from existing literature regarding its comparative analysis with the Haller index. This inclusion could provide readers with a clearer understanding of its relevance and utility from the outset.

Response 4: Thanks for your comments. I commented additional information from existing literature regarding its comparative analysis with the Haller index in “Validity of RPI for degree of PE” of result section and indicated the reference. “As in previous studies, we found no significant difference between the Haller index and RPI ( $p=0.431$ ) and a significant correlation between the Haller index and RPI ( $p<0.001$ ) (5,9,14)”. In addition, we commented that , measuring degree of chest wall depression by simple radiography could result in measurement errors that could be influenced by physiologic factors, especially in the asymmetric type in limitation section.

Comment 5: - To provide more context and transparency regarding the age groups, you may want to explain the rationale behind choosing the specific age cut-off of  $<10$  years versus  $\geq 10$  years for the division of subjects. This would help readers understand the reasoning behind this particular categorization.

Response 5: Thanks for raising an important issue. This is somewhat arbitrary, but we empirically divided the patient as age of ten (early vs. late repair). I published the paper titled as A cross-sectional study for the development of growth of patients with pectus excavatum (Eur J Cardiothorac Surg . 2016

Dec;50(6):1102-1109). This study showed that development of growth in patients with pectus excavatum is retarded and appears to be related to the severity of pectus excavatum. The development of growth can be recovered by early correction of the deformity. In addition, I published the paper titled as Recurrence of pectus excavatum following the Nuss procedure (J Thorac Dis . 2018 Nov;10(11):6201-6210.). This study shows that the effect of MIRPE is different according to the patient age at the time of the procedure. Early correction of PE can provide better corrective results because of the existence of a more pliable chest wall, which can be easily and sufficiently elevated by the MIRPE. Early correction means repair before age of ten.

Comment 6- Enhancing the transparency and credibility of the study could be achieved by providing detailed information about the surgical technique employed and by specifying the number of surgeons involved, along with their levels of experience in performing the procedures. This additional information would provide valuable context for the readers.

Response 6: Thanks for comments. I commented the surgical technique in our prior papers as references ... was conducted according to routine procedures at our institution (3,9).

Comments 7- Explaining the rationale for choosing the specific machine learning algorithms evaluated would strengthen this section.

Response 7: Thanks for your comments. I mentioned that "Performance scores of each model were calculated and evaluated based on area under the curve (AUC), accuracy, precision, F1 score, and recall. The outperformed model was selected based on AUC" in material and method section.

Comment 8:- Did you perform any variable selection process or feature engineering steps when developing the machine learning models to improve performance?

Response 8: We used The Orange® data mining toolbox for machine learning. The Orange® data mining toolbox in Python (Bioinformatics Lab at University of Ljubljana, Slovenia) was used for machine learning models learning (16). This open-source platform is a machine learning and data mining suite for data analysis through Python scripting and visual programming. the strongest is that we can use algorithms without coding process. The outperformed model was selected based on AUC. Indeed, we can get more better predictions using better coding or feature engineering techniques. However, we are not expert in coding or feature engineering techniques. Our study is feasible and simple technique for clinicians.

Comment 9:- Adding details on how categorical variables were encoded could clarify the model inputs.

Response 9: Categorical variable was age at the time of MIRPE, sex, RPI values, pectus deformity type (symmetric or asymmetric), number of inserted bars. These variables were all binary, which was explained by the manuscript.

Comment 10: Results: - The results are clearly presented. Adding a table to directly compare performance metrics across the machine learning models could help showcase the best performing prediction methods. Similarly, visualizations like prediction error plots could provide intuition on model performance.

Response 10: Thanks for comments. I provide additional tables as your comments (table 6 and 7).

Discussion:

Comment 11: Discussion- The discussion provides good clinical context for the study findings. Commenting on the generalizability of the models to other institutions could be useful for readers. Additionally, discussing model interpretability and features driving predictions would provide useful insight.

Response 11: Thanks for your comments. I revised the manuscript as your comments. I added the sentence "The generalizability of the models to other institutions should be studied" in Discussion sections. The external validation is needed. model interpretability and features are that "machine learning algorithms considering risk factors and basic clinical data yield good performance for prediction of final RPI and recurrence after BR. Such machine learning approaches can be convenient and provide accurate decisions in management of PE". These are commented in conclusion section.

Comment 12- Discussing requirements for clinical implementation could guide next steps for model validation.

Response 12: Thanks for your important feedback. We mentioned that "Because chest wall re-depression is

multifactorial and spatial, clinically available methods or modalities to evaluate and analyze chest wall re-depression are needed (19,20)”in discussion section. These tools are essential for better model validation. External validation should be performed in further studies.

Comment 13: conclusions-The conclusions accurately reflect the study findings. It would be helpful to reiterate the potential clinical utility of the models if validated in future studies.

Response 13: Thanks for your comments. I revised the manuscript as your comments. I added “ ...provide accurate decisions in management of PE..”

Comments 14: General- Consider expanding the abbreviations the first time they are introduced in the "Highlight Box" to ensure clarity for the readers.

Response 14. Thanks for your comments. The abbreviations in Highlight Box are all included in Explanatory legend.

Comments 15: With these additions, this well-conducted study could make a significant contribution to the literature on optimizing surgical care for patients with pectus excavatum.

Response 15: Thanks for your warm comments.

#### **Reviewer D**

Comment 1: Well written; interesting.

Response 1: Thanks for your warm comments.

#### **Reviewer E**

This is a paper that examined risk factors for recurrence after BR in patients with pectus excavatum who had undergone MIRPE. Since there is no universally accepted definition for recurrent pectus excavatum, the authors first established a definition for recurrent pectus excavatum. They then proceeded to track the course of recurrence and investigated risk factors for recurrence using machine learning. The Heller index, commonly used in the diagnosis of pectus excavatum, requires a CT scan, so the authors demonstrated the validity of the RPI, which can be measured using chest X-ray examinations, and employed RPI for imaging evaluation.

In conclusion, the authors used machine learning to predict recurrence as a function of parameters, including age group, sex, RPI values before and after MIRPE, pectus types (symmetric vs asymmetric), number of bars used, and angle of sternum. They demonstrated statistically significant results.

The core argument of the paper is valid, and I believe that utilizing machine learning for recurrence prediction, as the authors suggest, is worthy of publication. However, there are several areas that raise questions, so it would be advisable to include additional information in the discussion section.

Comment 1: It is indicated that RPI was higher in LG compared to EG before the MIRPE. RPI values can vary with age, and it is possible that even non-pectus excavatum patients have higher RPI values with increasing age. If there are previously published papers reporting the relationship between RPI and age, it would be advisable to include these references for further clarification.

Response 1: Thanks for your comments. The issue on the relationship between RPI and age is worthy of study as your comments. RPI is a key to this study and all analyses were performed by RPI. However, we did not include relationship between RPI and age in this study because the relationship between RPI and age is not defined. Stephen W. Daunt (Age-related normal ranges for the Haller index in children. *Pediatr Radiol* . 2004 Apr;34(4):326-30) reported there was no significant interaction of Haller index for age group and gender. Further studies should be needed.

Comment 2. If there is a possibility that RPI values may vary with age, it would be more appropriate to compare RPI values between LG and EG at the same age rather than within a consistent postoperative period. Is it feasible to conduct age-matched comparisons in the current study? Alternatively, do the authors have any insights or discussions on this matter?

Response 2: Thanks for your comments. I'm afraid I misunderstand your comments. We cannot compare the



RPI at the same age because the age between LG and EG were significantly different. In addition, the postoperative time were different according to age group. Atsushi Yoshida (Correlation of asymmetric chest wall deformity and growth in patients with pectus excavatum. *J Pediatr Surg* . 2013 Apr;48(4):771-5.) reported there was no significant correlation between Haller index and age. I think that age-matched comparisons cannot be performed in this study.

Comment 3. While I understand that the predictive ability of the machine learning model has been demonstrated, it is essential to provide details regarding whether other institutions, upon reading this report, can effectively establish predictions using the machine learning model. In other words, there is a need for further information on the practical applicability of the results from this study by other facilities.

Response 4: Thanks for your comments. We used The Orange® data mining toolbox for machine learning. The Orange® data mining toolbox in Python (Bioinformatics Lab at University of Ljubljana, Slovenia) was used for machine learning models learning (16). This open-source platform is a machine learning and data mining suite for data analysis through Python scripting and visual programming. the strongest is that we can use algorithms without coding process. We can perform prediction using RPI and other influencing factors in this study. We are not programmers, and we cannot develop the further better performance of algorithms without helps of experts. This is a pilot study on adoption of machine learning in pectus excavatum. Further studies should be needed for more performance of machine learning algorithms.

Comment 4. I would like to ask why you divided this study in 10 years of age. Now these days, many surgeons are thinking to start later than sooner. Do you comment on this?

Response 4. Thanks for your comments. Thanks for raising an important issue. This is also somewhat arbitrary, but we empirically divided the patient as age of ten (early vs. late repair). I published the paper titled as A cross-sectional study for the development of growth of patients with pectus excavatum (*Eur J Cardiothorac Surg* . 2016 Dec;50(6):1102-1109). This study showed that development of growth in patients with pectus excavatum is retarded and appears to be related to the severity of pectus excavatum. The development of growth can be recovered by early correction of the deformity. In addition, I published the paper titled as Recurrence of pectus excavatum following the Nuss procedure (*J Thorac Dis* . 2018 Nov;10(11):6201-6210.). This study shows that the effect of MIRPE is different according to the patient age at the time of the procedure. Early correction of PE can provide better corrective results because of the existence of a more pliable chest wall, which can be easily and sufficiently elevated by the MIRPE. Early correction means repair before age of ten. In addition, I think that early repair pectus excavation is better before puberty aggravation of pectus excavatum.