Error Indicators and Adaptive Refinement of Finite Element Thin-Plate Splines

Lishan Fang

Mathematical Sciences Institute
Australian National University

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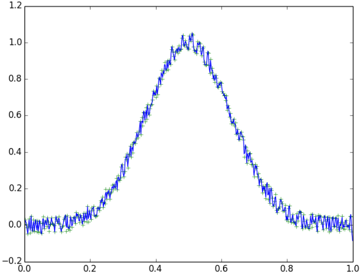
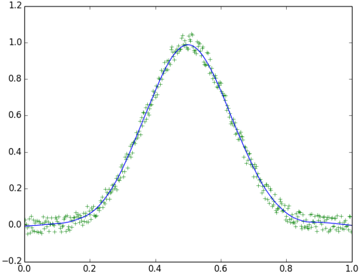
Outline

1. Finite element thin-plate splines
   - Thin-plate splines
   - Finite element representation
   - The $H^1(\Omega)$ method
   - 1D examples
2. Error indicator
   - Adaptive refinement
   - TPSFEM error indicator
   - Adaptively refined grids

Smooth data interpolation



(a) interpolating spline



(b) smoothing spline

Figure: $y = e^{-30(x-0.5)^2}$ with uniform noise [-0.05,0.05]

Thin-plate spline

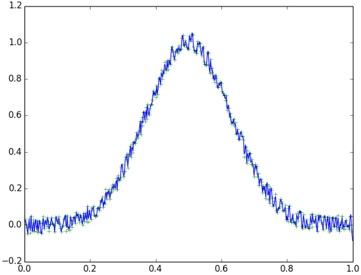
- Thin-plate spline (TPS) is a technique for interpolating and smoothing surface over scattered data [1].
- TPS smoother $f(\boldsymbol{x})$ predicts response values $y = f(\boldsymbol{x}) \in \mathbb{R}$ based on predictor values $\boldsymbol{x} \in \mathbb{R}^d$.
- Given n data points $\{(\boldsymbol{x}_{(i)}, y_{(i)}), i = 1, 2, ..., n\}$, TPS smoother $f(\boldsymbol{x})$ minimises

$$J_\alpha(f) = \frac{1}{n}\sum_{i=1}^{n}(f(\boldsymbol{x}_{(i)}) - y_{(i)})^2 + \alpha \int_\Omega \sum_{|v|=2} (D^v f(\boldsymbol{x}))^2 d\boldsymbol{x},$$

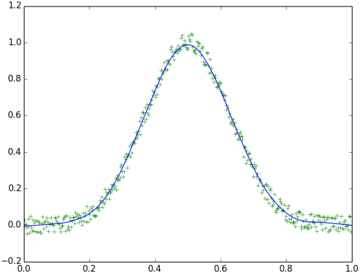
where α is the smoothing parameter.

[1] Buhmann, M.D., 2003. *Radial basis functions: theory and implementations (Vol. 12)*. Cambridge university press.

1D example: smoothing



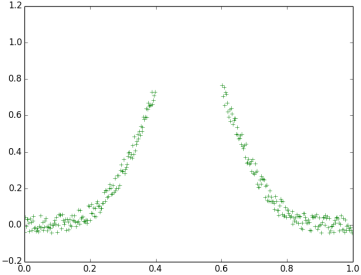
(a) $\alpha = 0$



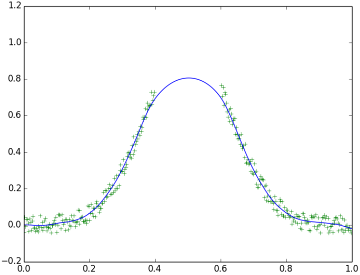
(b) $\alpha = 0.0001$

Figure: TPS interpolation

1D example: filling gaps



(a) data with a gap



(b) TPS with $\alpha = 0.0001$

Figure: TPS interpolation

Limitations

TPS requires a lot of storage for large datasets and is computationally expensive.

- System of equations is dense.
- Size of the system is proportional to the number of data points.

Example TPS approximations:

- compactly-supported radial basis functions;
- adaptive TPS;
- fast evaluation methods.

Finite element thin-plate splines

- Finite element thin-plate spline (TPSFEM) is a method that combines the finite element surface fitting and the TPS [1].
- TPSFEM smoother $s(\boldsymbol{x})$ is represented as a linear combination of piecewise linear basis functions

$$s(\boldsymbol{x}) = \boldsymbol{b}(\boldsymbol{x})^T \boldsymbol{c},$$

  where $\boldsymbol{b}$ are basis functions $\boldsymbol{b}(\boldsymbol{x}) = [b_1(\boldsymbol{x}), ..., b_m(\boldsymbol{x})]^T$ and $\boldsymbol{c}$ are coefficients of the basis functions.
- The size of the system depends on the number of basis functions instead of data points.

[1] Roberts, S., Hegland, M. and Altas, I., 2003. *Approximation of a thin plate spline smoother using continuous piecewise polynomial functions*. SIAM Journal on Numerical Analysis, 41(1), pp.208-234.

Recall

$$J_\alpha(f) = \frac{1}{n}\sum_{i=1}^{n}(f(\boldsymbol{x}_{(i)}) - y_{(i)})^2 + \alpha \int_\Omega \sum_{|v|=2} (D^v f(\boldsymbol{x}))^2 d\boldsymbol{x}.$$

Second order derivatives are not defined for piecewise linear basis functions $\boldsymbol{b}(\boldsymbol{x})$. Auxiliary functions $\boldsymbol{u}$ are introduced to represent the gradient of the smoother $s(\boldsymbol{x})$, where

$$\nabla s = \boldsymbol{u} = \begin{bmatrix} \boldsymbol{u}_1 \\ \ldots \\ \boldsymbol{u}_d \end{bmatrix} = \begin{bmatrix} \boldsymbol{b}(\boldsymbol{x})\boldsymbol{g}_1 \\ \ldots \\ \boldsymbol{b}(\boldsymbol{x})\boldsymbol{g}_d \end{bmatrix},$$

and $\boldsymbol{g}_1, \ldots, \boldsymbol{g}_d$ are coefficients to the basis representation of $\boldsymbol{u}_1, \ldots, \boldsymbol{u}_d$.

$s(\boldsymbol{x})$ and $\boldsymbol{u}$ satisfy the relationship

$$\int_\Omega \nabla s(\boldsymbol{x}) \nabla b_j(\boldsymbol{x}) d\boldsymbol{x} = \int_\Omega u(\boldsymbol{x}) \nabla b_j(\boldsymbol{x}) d\boldsymbol{x}$$

for every basis function $b_j(\boldsymbol{x})$. It is written as

$$L\boldsymbol{c} = \sum_{k=1}^{d} G_k \boldsymbol{g}_k,$$

where L is a matrix approximation to the negative Laplace operator ($L_{i,j} = \int_\Omega \nabla b_i \cdot \nabla b_j d\boldsymbol{x}$) and G_k is a matrix approximation to the gradient operator ($(G_k)_{i,j} = \int_\Omega b_i \cdot \partial_k b_j d\boldsymbol{x}$).

Discrete minimisation problem

The minimisation problem becomes

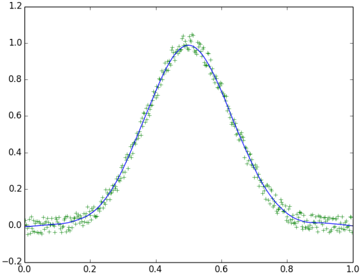
$$J_\alpha(\boldsymbol{c},\boldsymbol{g}) = \frac{1}{n}\sum_{i=1}^{n}(\boldsymbol{b}(x_{(i)})^T\boldsymbol{c} - y_{(i)})^2 + \alpha\int_\Omega \nabla\left(\boldsymbol{b}(x)^T\boldsymbol{g}\right)\nabla\left(\boldsymbol{b}(x)^T\boldsymbol{g}\right)dx$$

$$= \boldsymbol{c}^T A\boldsymbol{c} - 2\boldsymbol{d}^T\boldsymbol{c} + \boldsymbol{y}^T\boldsymbol{y}/n + \alpha\sum_{k=1}^{d}\boldsymbol{g}_{\boldsymbol{k}}^T L\boldsymbol{g}_{\boldsymbol{k}},$$

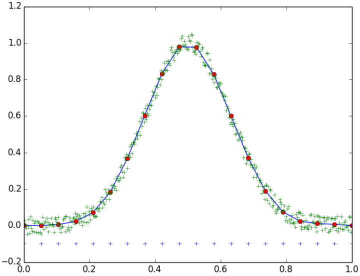
subject to $L\boldsymbol{c} = \sum_{k=1}^{d} G_k\boldsymbol{g}_k$, where

$$A = \frac{1}{n}\sum_{i=1}^{n}\boldsymbol{b}(x_{(i)})\boldsymbol{b}(x_{(i)})^T \quad \text{and} \quad \boldsymbol{d} = \frac{1}{n}\sum_{i=1}^{n}\boldsymbol{b}(x_{(i)})y_{(i)}.$$

1D example: smoothing



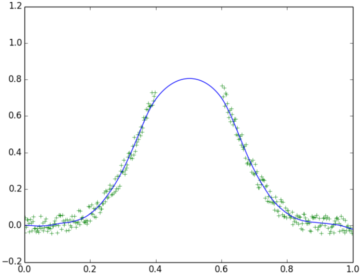
(a) TPS



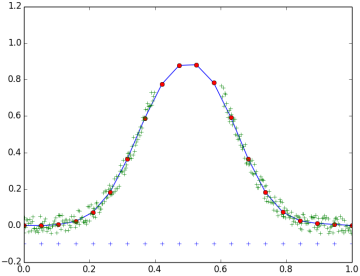
(b) TPSFEM with 20 nodes

Figure: $f(x) = e^{-30(x-0.5)^2}$ with uniform noise [-0.05,0.05]

1D example: filling gaps



(a) TPS



(b) TPSFEM with 20 nodes

Figure: $y = e^{-30(x-0.5)^2}$ with noise [-0.05,0.05] and a gap

Adaptive refinement

The accuracy of the finite element solution depends on the size of the finite element grid.

Uniform refinement is an approach to refine the whole region iteratively. But

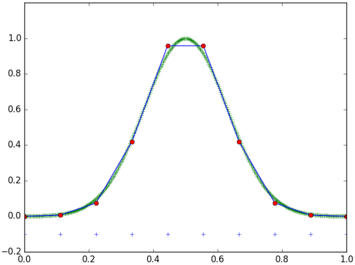
- high computational costs,
- high storage space.

Adaptive refinement adapt the precision of the solution within certain sensitive regions dynamically during the iterative refinement process [1]. E.g. peaks, boundaries, singularities.

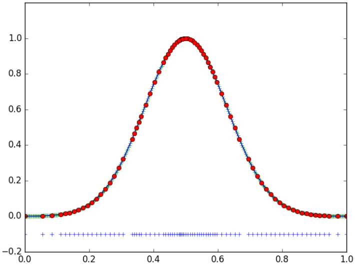
[1] Mitchell, W.F., 1989. *A comparison of adaptive refinement techniques for elliptic problems*. ACM Transactions on Mathematical Software (TOMS), 15(4), pp.326-347.

1D adaptive example

Assume function $f(x)$ is given, we can estimate the error using the true solution during the adaptive refinement process.



(a) initial grid

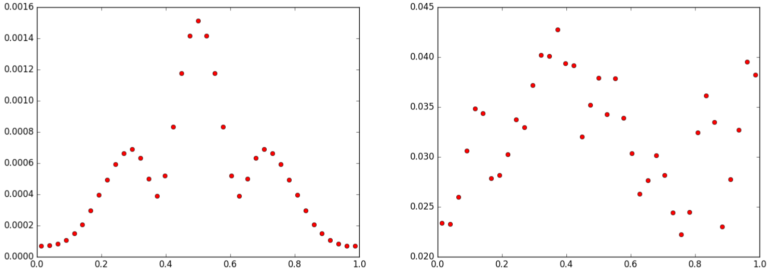


(b) adaptively refined grid

Figure: Adaptively refinement grids of $f(x) = e^{-30(x-0.5)^2}$

Regression metrics

In reality unction $f(x)$ is unknown but we can measure regression errors of the TPSFEM smoother against data points.



(a) no noise (b) uniform noise [-0.05,0.05]

Figure: Root mean squared error (RMSE) of $f(x) = e^{-30(x-0.5)^2}$ with 400 data points and 40 nodes

Challenges

Traditional error indicators of the FEM might not work for the TPSFEM:

- Error indicators are given different information.
- Data is usually perturbed by noise.
- Data are not uniformly distributed and some regions might not have any data.
- Error convergence of the TPSFEM depends on $\alpha + d^4 + h^4$, where α is the smoothing parameter, d is the minimum distance to any data point and h is the finite element mesh size.

Error indicator

Error indicators are methods that indicate large errors for elements in the finite element grid.

- Error estimate: estimate error bounds for the finite element solution in a specified norm.
- Error indicator: not necessarily estimate the error of the finite element solution.

Example finite element error indicators:

- auxiliary problem error indicator;
- recovery-based error indicator.

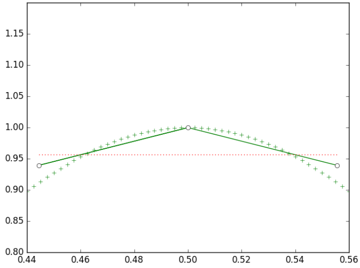
Auxiliary problem error indicator

- Estimate the error by comparing the current TPSFEM smoother with a more accurate solution.
- Approximate a more accurate local solution $\hat{\boldsymbol{s}}$ by solving the TPSFEM in a union of a smaller number of elements [1].
- The error is approximated by $||\hat{\boldsymbol{s}} - \boldsymbol{s}||$.
- Determine the space for improvement in accuracy instead of estimating the error directly.
- Higher accuracy
  - higher order polynomial,
  - refine the elements with the same order polynomial.

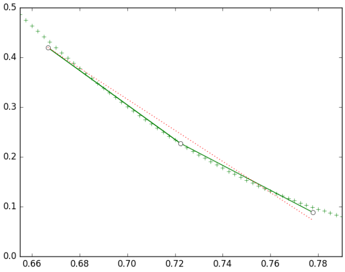
[1] Mitchell, W.F., 1989. *A comparison of adaptive refinement techniques for elliptic problems*. ACM Transactions on Mathematical Software (TOMS), 15(4), pp.326-347.

Auxiliary problem examples

- Dotted line is the current TPSFEM smoother.
- Solid line is the local solution.



(a) large error



(b) small error

Recovery-based error indicator

- Calculates the error norm by post-processing the discontinuous gradients across interelement boundaries [1].
- The improved gradient $\hat{\nabla} s_i$ is determined by

$$\sum_{i=1}^{n} \int_{\Omega} b_j b_i \hat{\nabla} s_i d\Omega = \int_{\Omega} b_j \nabla s d\Omega, \qquad j = 1, ..., m, \tag{1}$$

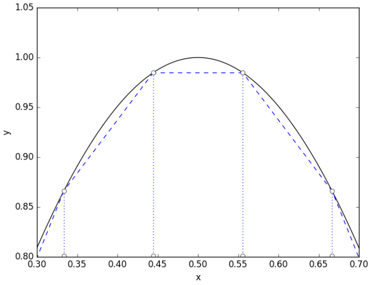
  where ∇s is the current gradient.
- The error is estimated by

$$||e||_E^2 \approx \int_{\Omega} (\hat{\nabla} s - \nabla s)^2 d\Omega. \tag{2}$$

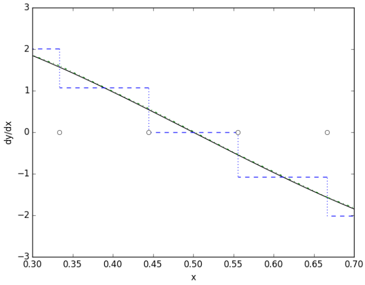
[1] Zienkiewicz, O.C. and Zhu, J.Z., 1987. A simple error estimator and adaptive procedure for practical engineering analysis. International journal for numerical methods in engineering, 24(2), pp.337-357.

Discontinuous gradient

- Dashed line is the current TPSFEM approximation.
- Solid line is the true model problem solution.
- Dash-dotted line is the improved gradient.



(a) FE approximation



(b) gradient discontinuities

Model problem

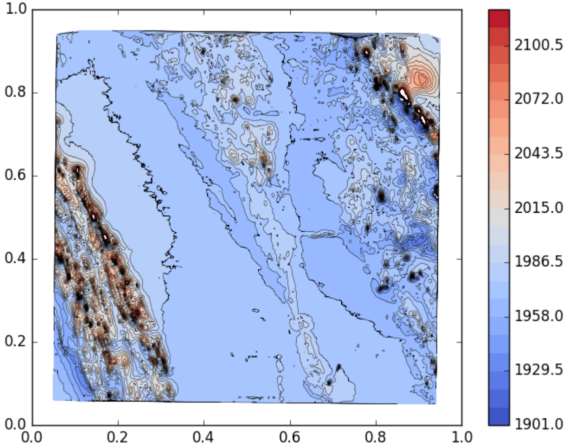
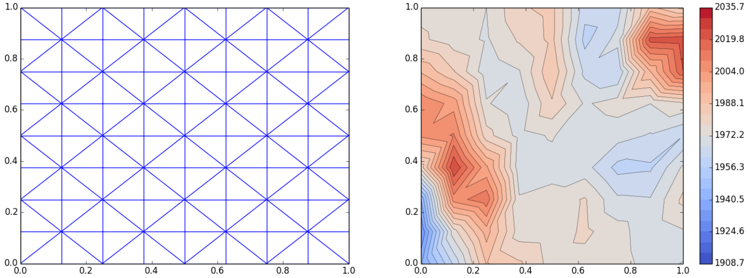


Figure: Ebagoola magnetic dataset of 735700 points with latitude, longitude and magnetic field strength

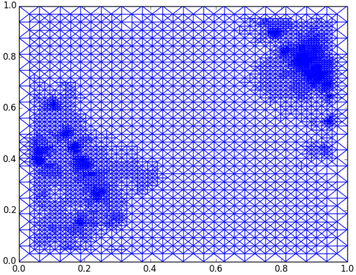
Initial TPSFEM smoother



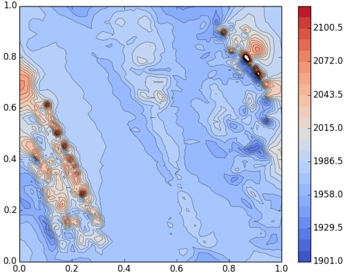
(a) FE grid with 81 nodes (b) smoother with error 20.34

Figure: Initial TPSFEM smoother before refinement

Adaptively refined grids I

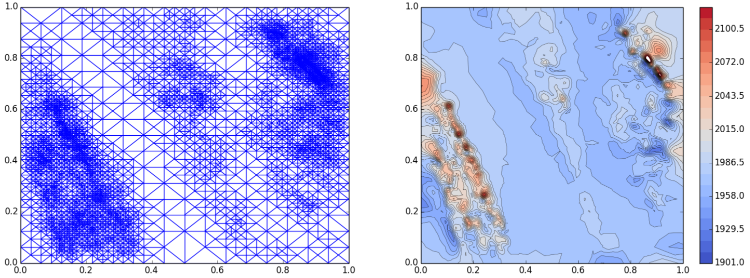


(a) FE grid with 5540 nodes



(b) smoother with error 5.83

Figure: Adaptively refined TPSFEM smoother using the auxiliary problem error indicator



(a) grid with 5440 nodes

(b) smoother with error 5.69

Figure: Adaptively refined TPSFEM smoother using the recovery-based error indicator

Limitations

- Auxiliary problem error indicator:
  - Require high computational costs and memory requirement.
  - May lead to over-refinement due to noise.
- Recovery-based error indicator
  - May not detect smaller trends in data that are not modeled by the finite element grid.

Future research

- Address the influence of α and *d*.
- Test error indicators with datasets with different model problems, distributions and noises.
- Adaptive smoothing of the TPSFEM.

References

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