### Interpolants, Error Bounds, and Mathematical Software for Modeling and Predicting Variability in Computer Systems



# Chapters

### 1. The Importance and Applications of Variability

- 2. Algorithms for Constructing Approximations
- 3. Naive Approximations of Variability
- 4. Box-Splines: Uses, Constructions, and Applications
- 5. Stronger Approximations of Variability
- 6. An Error Bound for Piecewise Linear Interpolation
- 7. A Package for Monotone Quintic Spline Interpolation



# What is "Variability"?

### A *random variable* uniquely defined by its Cumulative Distribution Function (CDF) / Probability Density Function (PDF)



З



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# Variability in Systems

When the same computer is used to execute the same program repeatedly, most measurable performance characteristics will vary.





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Managing this performance variability can be very important in applications where we want to meet some set requirements.



### VarSys: Modeling and Managing Variability



#### **High Performance Computing**

HPC systems consume a lot of energy and time, both are functions of how the system was built and configured. Models can be used to optimize a configuration.

#### **Cloud Computing**

Small savings in compute time and performance magnify greatly when 1000's of machines are involved. Service Level Agreements (SLAs) can be tightened.

#### **Computer Security**

A strong understanding of variability can improve defenses against malicious users by demonstrating new vulnerabilities, and helping prevent side channel attacks.



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### Variability is important in many aspects of computation.



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Variability is important in many aspects of computation.

Quantifying variability and constructing models of it may lead to improvements in all of these aspects of computation.



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Given

underlying function  $f : \mathbb{R}^{d} \to \mathbb{R}$ data matrix  $X^{d \times n}$  with column vectors  $x^{(i)} \in \mathbb{R}^{d}$ function values  $f(x^{(i)})$  for all  $x^{(i)}$ vector f(X) has elements  $f(x^{(i)})$ 





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Regression  $\hat{f}_p$  has parameters p and is the solution to  $\min_p \| \hat{f}(X) - f(X) \|$ 





#### Multivariate Adaptive Regression Splines

$$B_{2j-1}(x) = B_l(x) (x_i - x_i^{(p)})_+$$
$$B_{2j}(x) = B_k(x) (x_i - x_i^{(p)})_-$$

### Multilayer Perceptron Regressor

$$p(x) = \sum_{i=1}^{n} a_i K(x, x^{(i)}) + b$$

$$l(u) = \left(u^t W_l + c_l\right)_+$$









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Delaunay

#### **Modified Shepard**

Linear Shepard

simplicial mesh

squared inverse distance

local linear fit

$$y = \sum_{i=0}^{d} w_i x^{(i)}, \quad \sum_{i=0}^{d} w_i = 1, \quad w_i \ge 0, \quad i = 0, \dots, d$$
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$$p(x) = \frac{\sum_{k=1}^{n} W_k(x) f(x^{(k)})}{\sum_{k=1}^{n} W_k(x)}$$









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# IOzone – A System Benchmark

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#### **System Specs:**

Two Intel Xeon E5-2637 CPUs with total 16 CPU cores and 16GB DRAM per node, at 12 nodes.

Ext4 filesystem above an Intel SSDSC2BA20 SSD drive.

Each of ~20K unique system configurations were run 150 times.

System Parameter	Values
File Size (KB)	4, 16, 64, 256, 1024, 4096, 8192, 16384
Record Size (KB)	4, 8, 16, 32, 64, 128, 256, 512, 1024, 2048, 4096, 8192, 16384
Thread Count	1, 8, 16, 24, 32, 40, 48, 56, 64
Frequency (GHz)	1.2, 1.6, 2, 2.3, 2.8, 3.2, 3.5
Test Type	Readers, Rereaders, Random Readers, Initial Writers, Rewriters, Random Writers



# **Mean Prediction Results**





# Variance Prediction Results





## **Chapter Takeaways**

Multivariate models of HPC system performance can predict I/O throughput mean and variance.

The Delaunay method produces considerably better results for mean and variance prediction.

Throughput variance is harder to predict than mean throughput.



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# **Box Splines**

Proposed by C. de Boor as an extension of B-Splines into multiple dimensions (without using tensor products).

Can be shifted and scaled without losing smoothness.

Computationally expensive.





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# **Testing and Evaluation: Data**



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High Performance Computing File I/O n = 532, d = 4predicting file I/O throughput




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High Performance Computing File I/O n = 532, d = 4predicting file I/O throughput

Forest Fire n = 517, d = 12predicting *area burned* 





# **Testing and Evaluation: Data**

High Performance Computing File I/O n = 532, d = 4predicting file I/O throughput

Forest Fire n = 517, d = 12predicting *area burned* 

Parkinson's Clinical Evaluation n = 468, d = 16predicting total clinical "UPDRS" score





# Average Relative Testing Error (y-axis) versus Relative Error Tolerance (x-axis)





#### **Chapter Takeaways**

The "Max" method appears to produce better results than the "Iterative" method. The Voronoi Cell method is best for I/O, but worst for all other tests.

The bootstrapping combined with the least squares computation incurs a lot of computational expense. This methodology **cannot be scaled** to more than 100's of points.



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# **Interpolating Distributions**

A Cumulative Distribution Function (CDF)  $F : \mathbb{R} \to \mathbb{R}$ must maintain the properties:

 $F(x) \in [0,1]$ 

F(x) is absolutely continuous and nondecreasing.

A convex combination of CDFs results in a valid CDF. Consider this example, solid line is the weighted sum:

{.3 Red, .4 Green, .3 Blue}





# **Measuring Error in a Prediction**

Kolmogorov Smirnov (KS) statistic, max-norm difference.

Null hypothesis (of distributions being same) is rejected at confidence level *p* according to  $KS > \sqrt{-\frac{1}{2}\ln\left(\frac{p}{2}\right)}\sqrt{\frac{1}{n_1} + \frac{1}{n_2}}$ 

Dotted lines – source CDFs

Dashed line – predicted CDF (Delaunay)

Solid line – true CDF

Red arrow – KS statistic between predicted and true (.2)





# **Results Applied to IOzone**

x-axis – KS Statistic y-axis – Number of predictions

Red lines: KS significance levels at {.1.05, .01, .001}

Consider all values to the right of a red line an "incorrect" prediction at that significance.



# **Increasing Training Data**

x-axis – Percentage training data y-axis – Percentage N.H. rejections Below: Aggregate Right: Breakdown by Test





# Improving Performance with Tuning

Algorithm	P-Value	Unweighted % N.H. Rejection	Weighted % N.H. Rejection
Delaunay		24.9	30.2
Max Box Mesh	.05	21.3	21.2
Voronoi Mesh		18.7	11.3
Delaunay		21.6	27.4
Max Box Mesh	.01	16.4	16.4
Voronoi Mesh		14.9	7.0
Delaunay		19.7	25.4
Max Box Mesh	.001	13.1	13.1
Voronoi Mesh		12.3	4.6
Delaunay		17.9	23.4
Max Box Mesh	1.0e-6	11.3	11.3
Voronoi Mesh		8.5	2.3

Consensus optimal weighting of (.001, 2, 1.7, 1.5), for frequency, file size, record size, and number of threads. Frequency is unimportant.

#### **Chapter Takeaways**

Without any modification, many interpolants can be used to predict distributions! Particularly, those that make predictions with convex combinations of known function values.

Distribution prediction performs well, impressively so with tuning (however the tuning is less provably useful).

20K system configurations appears to approach the limit of distribution prediction accuracy. If we had a better way to approximate distributions, we might reduce error further.



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$$\left| f(z) - \hat{f}(z) \right| \le \frac{\gamma \|z - x_0\|_2^2}{2} + \frac{\sqrt{d\gamma k^2}}{2\sigma_d} \|z - x_0\|_2$$



$$|f(z) - \hat{f}(z)| \le \frac{\gamma \|z - x_0\|_2^2}{2} + \frac{\sqrt{d\gamma k^2}}{2\sigma_d} \|z - x_0\|_2$$

The absolute error of a linear interpolant is tightly upper bounded by



$$|f(z) - \hat{f}(z)| \le \frac{\gamma ||z - x_0||_2^2}{\uparrow 2} + \frac{1}{2}$$

$$\frac{\|2}{2} + \frac{\sqrt{d\gamma k^2}}{2\sigma_d} \|z - x_0\|_2$$

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/ 1

The absolute error of a linear interpolant is tightly upper bounded by

the max change in slope of the function



$$|f(z) - \hat{f}(z)| \le \frac{\gamma ||z - x_0||_2^2}{2} + \frac{\sqrt{d\gamma k^2}}{2\sigma_d} ||z - x_0||_2$$

The absolute error of a linear interpolant is tightly upper bounded by

the max change in slope of the function

times the distance to the nearest known point squared







$$\begin{split} \left| f(z) - \hat{f}(z) \right| &\leq \frac{\gamma \|z - x_0\|_2^2}{2} + \frac{\sqrt{d} \gamma k_*^2}{2\sigma_d} \|z - x_0\|_2 \\ \end{split}$$
The absolute error of a linear interpolant is tightly upper bounded by
the max change in slope
plus the square root of the dimension times the max change in slope
times the longest edge length between points defining the linear interpolant squared
the dimension times the max change in slope
times the longest edge length between points defining the linear interpolant squared







### The Importance

The approximation error of a linear (simplicial) interpolant tends quadratically towards zero when approaching observed data only when the diameter of the simplex is also reduced proportionally.

In practice, only linear convergence to the true function can be achieved (because the evaluation points don't move).

Approximation error is largely determined by **data spacing**!

This theory only directly applies to Delaunay, but may give insight into the approximation behavior of other techniques.



#### **Piecewise Linear Approximations**

#### Delaunay (interpolant)

$$y = \sum_{i=0}^{d} w_i x^{(i)}, \quad \sum_{i=0}^{d} w_i = 1, \quad w_i \ge 0, \quad i = 0, \dots, d$$
$$\hat{f}(y) = \sum_{i=0}^{d} w_i f(x^{(i)})$$

Multilayer Perceptron (regressor)

$$l(u) = \left(u^t W_l + c_l\right)_+$$







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# Approximating $f(x) = \cos(||x||_2)$

In 2 dimensions, we get expected results. Delaunay is better at interpolation, MLP better at regression.



Approximating  $f(x) = \cos(||x||_2)$ 

In 20 dimensions, the *intuitive* trend disappears! Delaunay and MLP look the same.



#### **Explaining the Convergence**



### **Connecting Back to Theory**

$$|f(z) - \hat{f}(z)| \le \frac{\gamma ||z - x_0||_2^2}{2} + \frac{\sqrt{d\gamma k^2}}{2\sigma_d} ||z - x_0||_2$$



### **Connecting Back to Theory**





### **Connecting Back to Theory**





# **Data Sets for Empirical Evaluation**

Forest Fire (n = 504, d = 12)

given meteorological information about a park, predict the amount of land that would be burned in a forest fire.

Parkinson's Telemonitoring (n = 5875, d = 19) given features of audio recorded in the home of someone with Parkinson's, predict their next clinical evaluation score.

- Australian Daily Rainfall Volume (n = 2609, d = 23) given meteorological data around Sydney, Australia, predict the amount of rainfall that will occur on the next day.
- Credit Card Transaction Amount (n = 5562, d = 28) given anonymized electronic transaction features (output of PCA) predict the amount of money that the transaction will process.

High Performance Computing I/O (n = 3016, d = 4) given system configuration information, predict the distribution of I/O throughput that will be seen at a new configuration.



Forest fire data





Parkinson's Telimonitoring





Australian Rainfall





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**Credit Card Transactions** 





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**IOzone Distribution Models** 





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### **Chapter Takeaways**

Interpolants have provable convergence properties.

Interpolants produce competitive approximations in medium dimension, while requiring very little "fit" time.

Some interpolants easily generalize to predicting functions.

Algorithm	Avg. % Best	Avg. Fit or Prep. Time (s)	Avg. App. Time (s)
MARS	4.5	$20.0\mathrm{s}$	0.001s
$\operatorname{SVR}$	19.5	$\mathbf{0.5s}$	$\mathbf{0.0001s}$
$\operatorname{MLP}$	43.1	200.0s	$0.001\mathrm{s}$
Delaunay	5.2	1.0s	1.0s
$\operatorname{ShepMod}$	18.0	$0.7\mathrm{s}$	$\mathbf{0.0001s}$
LSHEP	8.4	$2.0\mathrm{s}$	$\mathbf{0.0001s}$
Voronoi	0.5	1.0s	$0.04 \mathrm{s}$
BoxSplines	3.5	0.8s	$0.0005\mathrm{s}$



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## **Connection to Variability**



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## **Monotone Piecewise Quintic Splines**

Theory existed to create splines that are composed of quintics, but no mathematical software had been produced!

G. Ulrich and L. Watson. Positivity conditions for quartic polynomials. SIAM Journal on Scientific Computing, 15(3):528–544, 1994. doi: 10.1137/0915035. URL https://doi. org/10.1137/0915035.

Walter Hess and Jochen W Schmidt. Positive quartic, monotone quintic c2-spline interpolation in one and two dimensions. Journal of Computational and Applied Mathematics, 55(1): 51–67, 1994. doi: 10.1016/0377-0427(94)90184-8.

Dougherty, Randall L., Alan S. Edelman, and James M. Hyman. Nonnegativity-, monotonicity-, or convexity-preserving cubic and quintic Hermite interpolation. Mathematics of Computation 52.186 (1989): 471-494.



### Proposed Software Package, MQSI

Algorithm 1: QUADRATIC\_FACET(X(1:n), Y(1:n), i)

where  $X_j, Y_j \in \mathbb{R}$  for  $j = 1, ..., n, 1 \leq i \leq n$ , and  $n \geq 3$ . Returns the slope and curvature at  $X_i$  of the local quadratic interpolant with minimum magnitude curvature.

#### Algorithm 2:

IS\_MONOTONE $(x_0, x_1, f(x_0), Df(x_0), D^2f(x_0), f(x_1), Df(x_1), D^2f(x_1))$ where  $x_0, x_1 \in \mathbb{R}, x_0 < x_1$ , and f is an order six polynomial defined by  $f(x_0)$ ,  $Df(x_0), D^2f(x_0), f(x_1), Df(x_1), D^2f(x_1)$ . Returns TRUE if f is monotone increasing on  $[x_0, x_1]$ .

#### Algorithm 3: MQSI(X(1:n), Y(1:n))

where  $(X_i, Y_i) \in \mathbb{R} \times \mathbb{R}$ , i = 1, ..., n are data points. Returns monotone quintic spline interpolant Q(x) such that  $Q(X_i) = Y_i$  and is monotone increasing (decreasing) on all intervals that  $Y_i$  is monotone increasing (decreasing).



#### Some examples





## MQSI given difficult data



ICE

#### **Approximating VarSys Data**





#### Measuring Accuracy, a Test





















### The Quintic is Often Better for Tested VarSys Data



#### **Approximating VarSys Data**





# The Big Picture

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## Publications along the way

T. C. H. Lux, T. H. Chang, L. T. Watson, J. Bernard, B. Li, L. Xu, G. Back, A. R. Butt, K. W. Cameron, and Y. Hong, "Predictive modeling of I/O characteristics in high performance computing systems", in Proc. 2018 Spring Simulation Multiconference, 26th High Performance Computing Symp., L. T. Watson, W. I. Thacker, M. Sosonkina, J. Weinbub, and K. Rupp (eds.), Soc. for Modelling and Simulation Internat., Vista, CA, 2018, 434–445.

Thomas C. H. Lux, Layne T. Watson, Tyler H. Chang, Jon Bernard, Bo Li, Xiaodong Yu, Li Xu, Godmar Back, Ali R. Butt, Kirk W. Cameron, Danfeng Yao, and Yili Hong. 2018. Novel meshes for multivariate interpolation and approximation. In Proceedings of the ACMSE 2018 Conference (ACMSE '18). ACM, New York, NY, USA, Article 13, 7 pages. DOI: <u>https://doi.org/</u><u>10.1145/3190645.3190687</u>

Thomas C. H. Lux, Layne T. Watson, Tyler H. Chang, Jon Bernard, Bo Li, Xiaodong Yu, Li Xu, Godmar Back, Ali R. Butt, Kirk W. Cameron, Danfeng Yao, and Yili Hong. 2018. Nonparametric Distribution Models for Predicting and Managing Computational Performance Variability. In Proceedings of the IEEE SoutheastCon 2018 Conference (IEEESE '18). IEEE, Tampa, FL, USA, 7 pages.

T. C. H. Lux, L. T. Watson, T. H. Chang, Y. Hong, K. C. Cameron (2019) Interpolation of Sparse High-Dimensional Data. Springer Numerical Algorithms.

Lux, T.C.H., Chang, T.H. & Tipirneni, S.S. Least-squares solutions to polynomial systems of equations with quantum annealing. Quantum Inf Process 18, 374 (2019). <u>https://doi.org/10.1007/s11128-019-2489-x</u>

T. C. H. Lux, S. Nagy, M. Almanaa, S. Yao and R. Bixler, "A Case Study on a Sustainable Framework for Ethically Aware Predictive Modeling," 2019 IEEE International Symposium on Technology and Society (ISTAS), Medford, MA, USA, 2019, pp. 1-7.

Thomas C. H. Lux, Layne T. Watson, Tyler H. Chang, Li Xu, Yueyao Wang, Yili Hong. An Algorithm for Constructing Monotone Quintic Interpolating Splines. Spring Simulation Multiconference, High Performance Computing Symposium. February, 2020.

Thomas C. H. Lux, Layne T. Watson, Tyler H. Chang, Li Xu, Yueyao Wang, Jon Bernard, Yili Hong, Kirk W. Cameron. Effective Nonparametric Distribution Modeling for Distribution Approximation Applications. Institute of Electrical and Electronics Engineers Southeastcon. January, 2020.

Thomas C. H. Lux, Tyler H. Chang. Analytic Test Functions for Generalizable Evaluation of Convex Optimization Techniques. Institute of Electrical and Electronics Engineers Southeastcon. January, 2020.

Thomas C. H. Lux, Layne T. Watson, Tyler H. Chang, William I. Thacker. Algorithm XXXX: MQSI—Monotone Quintic Spline Interpolation. ACM Transactions on Mathematical Software. Planning to submit August, 2020.



# Publications along the way

#### Contributed

#### Chapters

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- T. C. H. Lux, T. H. Chang, L. T. Watson, J. Bernard, B. Li, L. Xu, G. Back, A. R. Butt, K. W. Cameron, and Y. Hong, "Predictive modeling of I/O characteristics in high performance computing systems", in Proc. 2018 Spring Simulation Multiconference, 26th High Performance Computing Symp., L. T. Watson, W. I. Thacker, M. Sosonkina, J. Weinbub, and K. Rupp (eds.), Soc. for Modelling and Simulation Internat., Vista, CA, 2018, 434–445.
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# Overview

- 1. The Importance and Applications of Variability define variability, why is it important?
- 2. Algorithms for Constructing Approximations approximation, regression and interpolation techniques
- 3. Naive Approximations of Variability mean, variance, and standard deviation prediction with IOzone
- 4. Box-Splines: Uses, Constructions, and Applications spline overview, box splines, meshes, fitting, and data sets
- 5. Stronger Approximations of Variability predicting distributions, measuring error, and tuning
- 6. An Error Bound for Piecewise Linear Interpolation theoretical bound, synthetic demo, and empirical results
- 7. A Package for Monotone Quintic Spline Interpolation MQSI algorithms, example pictures, performance study

