Beyond Design of Experiments (DOE)

Selden Crary, Palo Alto

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Acknowledgments

Optimal design-of-experiments co-authors[1]:

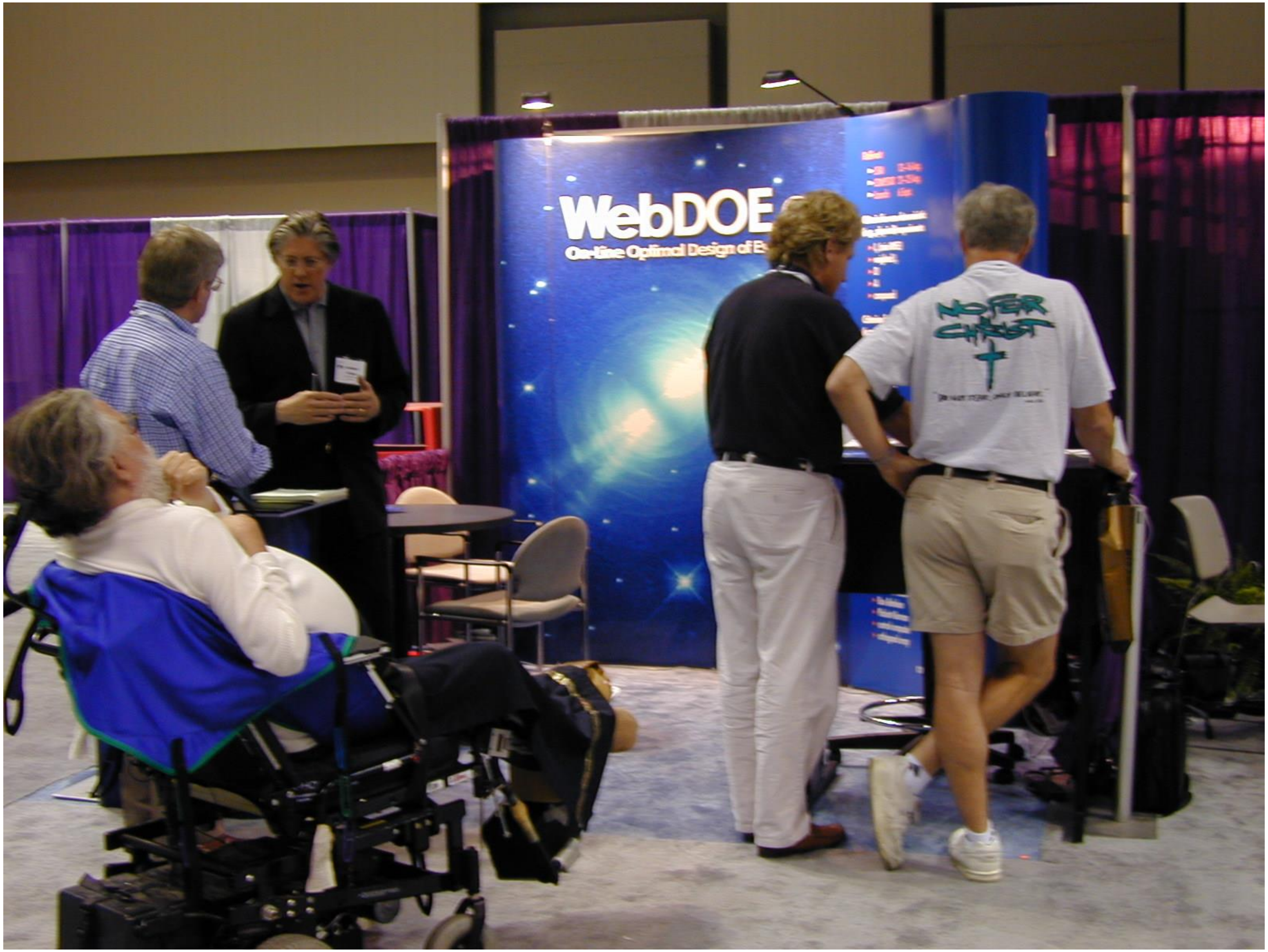
Physical experiments: Wayne Baer, John Cowles, Kensall Wise, Mark Sherwin, Gordon Munns, Michael Elta, E. G. Woelk, Fred Terry, George Haddad, Ling Hoo, Mark Tennenhouse, Mark Snow, Cosimo Spera, Peter Cousseau, David Armstrong, Eva Mok, Olivier Dubochet, Philippe Lerch, Philippe Renaud, Yousceek Jeong, Hee-Jung Lee, Bachar Affour, David Bernstein, Yogesh Gianchandani, and Mary Ann Maher.

Twin-point designs for computer experiments: David Woodcock, Andreas Hieke, Rachel Johnson, Jan Stormann, Tatiana Nizhegorodova, Michael Saunders, Richard Diehl Martinez, Amin Mobasher, and Nikoloz Chkonia.

Special thanks to: Linda Haines (U. Pietermaritzburg, now Cape Town), Pinaki Mazumder (U. Mich., Ann Arbor), Fred Hickernell (Illinois Inst. Tech.), Bradley Jones (SAS/JMP), Hermann Schichl (U. Vienna), Avery Bedows, Bruce Pourciau (Lawrence U.), Max Morris (Iowa St. U.), and Graham Gyatt.

[1]Paper list: https://seldencrary.com/pubs/


Selden
Crary
Dr. Andreas
Hieke
Design of Exper



Dave Woodcock (seated), Univ. Michigan Systems Programmer extraordinaire & co-discoverer of twin-point designs, observing the action at the WebDOE™ booth at JSM 2000. The WebDOE logo hinted at possible physics connections of twin-point designs.

Amin Mobasher
former S'ford EE postdoc
who finds time …

Avery Bedows
Founder/CEO
Altar Virtual Technologies

Jan Stormann
Vienna high-schooler
now ETH/Zurich

With Stanford Prof. Michael Saunders and Stanford graduate student Richard Diehl Martinez.

Sharing a meal in Auburn, CA with composite-particle researcher Walt Perkins, who asked of twin points, “So those are your strings?”

Outline

Part 1. Four surprises in optimal DOE, including
availability of free software

Part 2. Six objections to twin-points, including
twin-point designs w/o higher precision

Part 3. Think the unthinkable
DOE $\leftrightarrow$ QFT ?

Q&A

References

Surprise #1

Surprise #1

High-school chemistry experiment

Determine the activation energy E_a for a specific chemical reaction.

- The temperature dependence of the rate of many chemical reactions follows the Arrhenius equation:

$$k = Ae^{-E_a/RT}$$

- Assume A, E_a, and R are constant.
- At 10 fixed T's: Record T & k (the mass of solid produced)
- Determine E_a and its uncertainty.

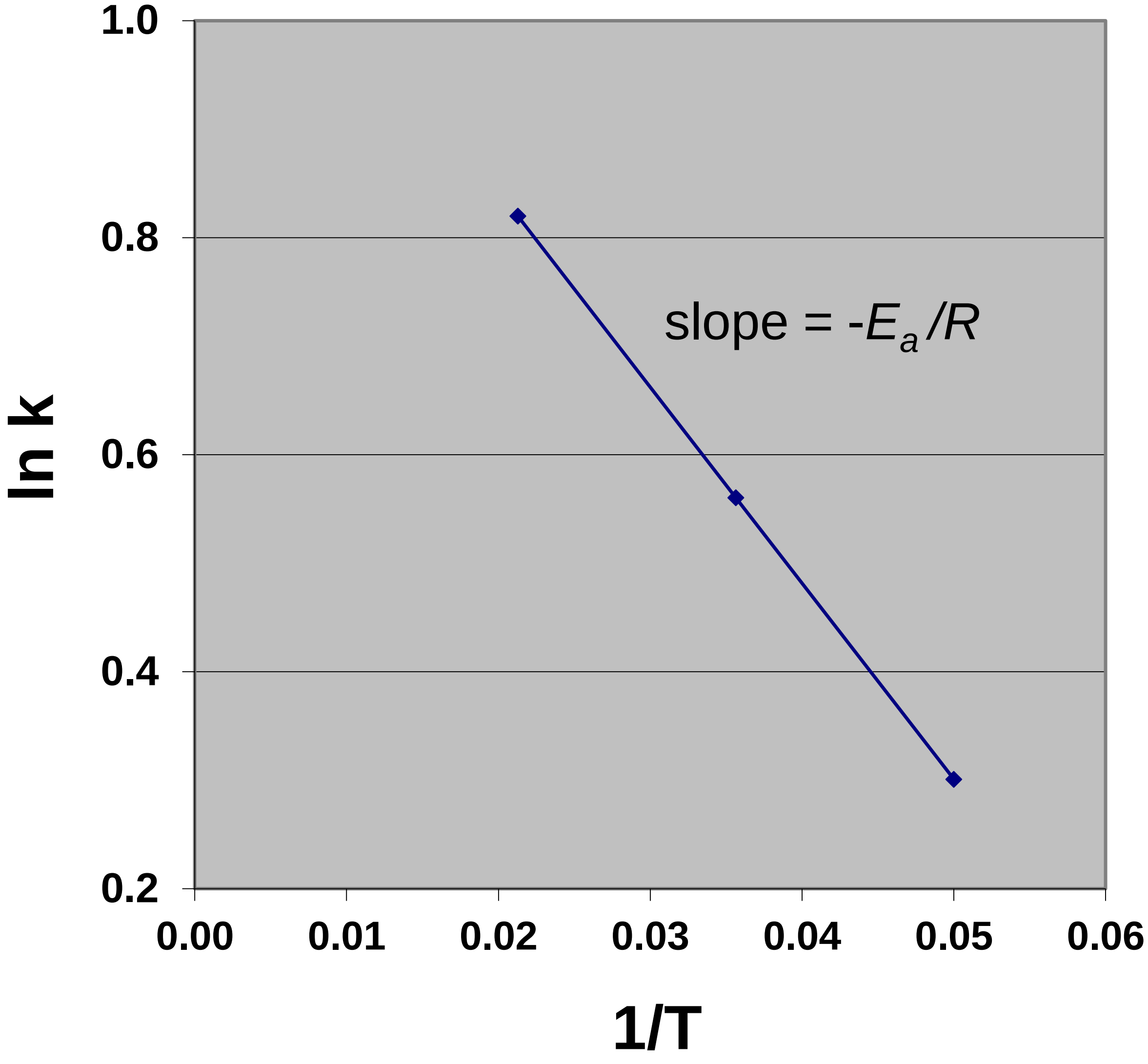
Surprise #1

$$k = Ae^{-E_a/RT}$$

$$\ln k = \ln A - \frac{E_a}{RT}$$

$$\text{Plot } \ln k \ vs. \ \frac{1}{T}$$

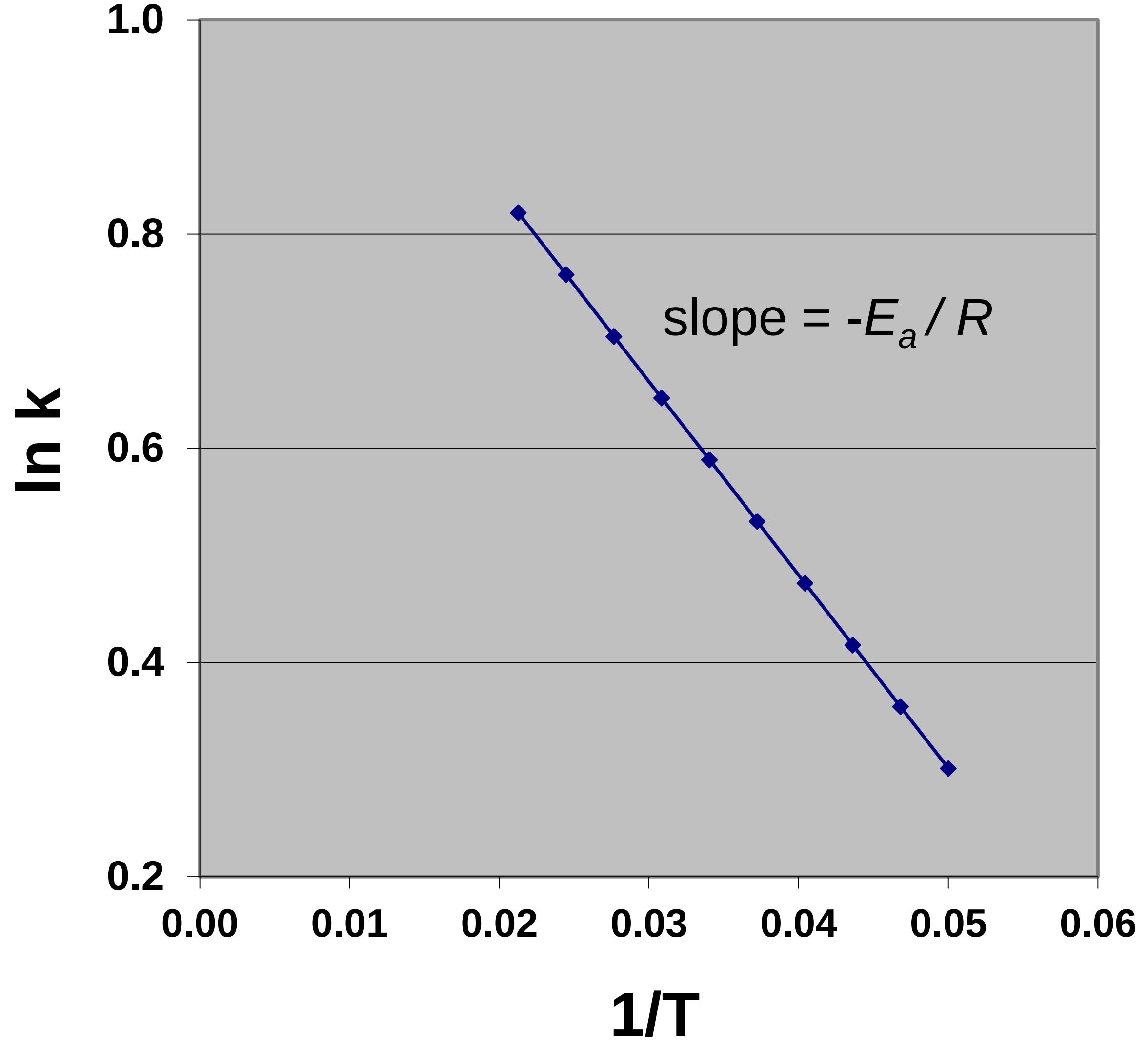
Surprise #1



Surprise #1

- Student: “How should we space the points?”
- Teacher: “What do you mean?
- Student: “What temperatures should we use?
- Teacher: “Take them evenly spaced.”

Surprise #1



Surprise #1

- The teacher’s advice, “Take them evenly spaced” was a puzzle for the student for 25 years, until he learned about DOE.

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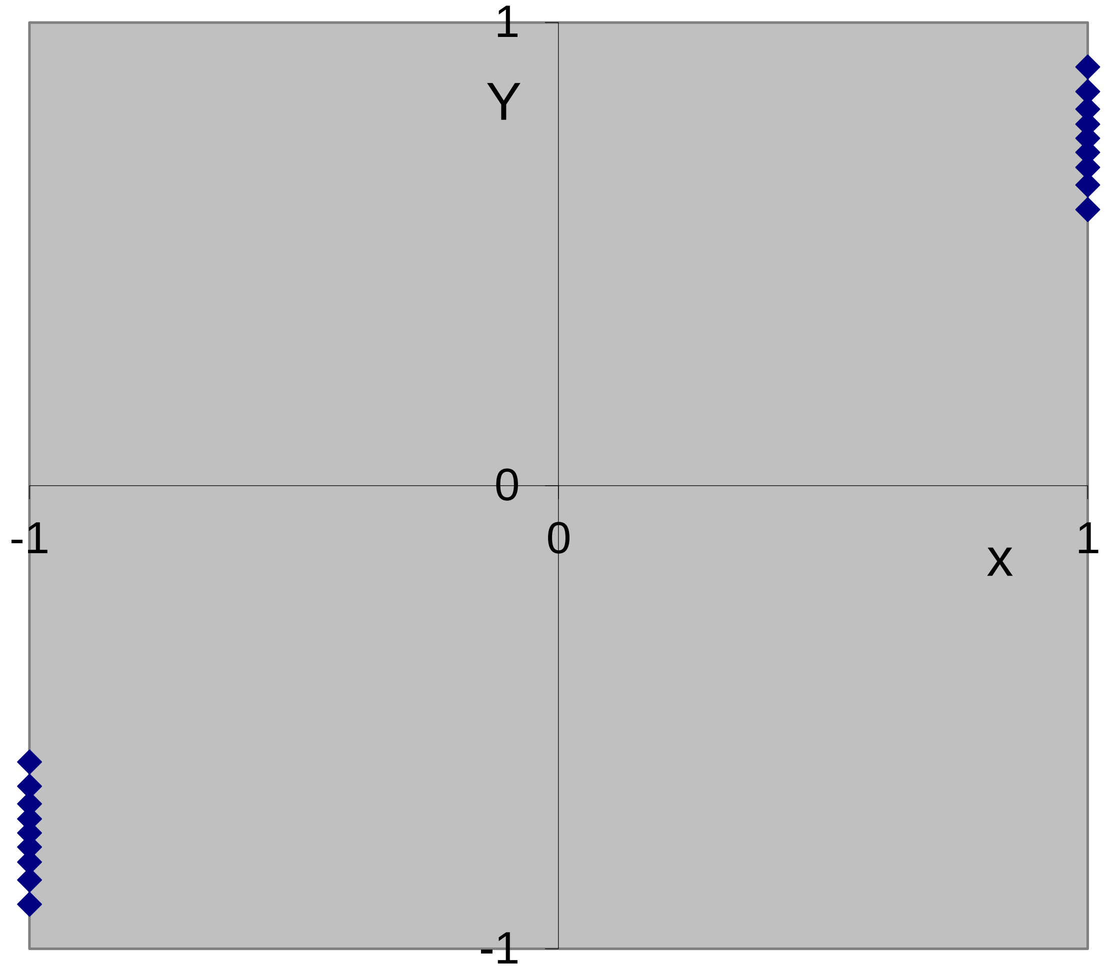
Surprise #1

- The teacher's advice, "Take them evenly spaced" was a puzzle for the student for 25 years, until he learned about DOE.
- Ten evenly spaced trials worked fine.
- But, taking the trials at the ends of the T interval would have (likely) given a smaller uncertainty in E_a, as we now discuss.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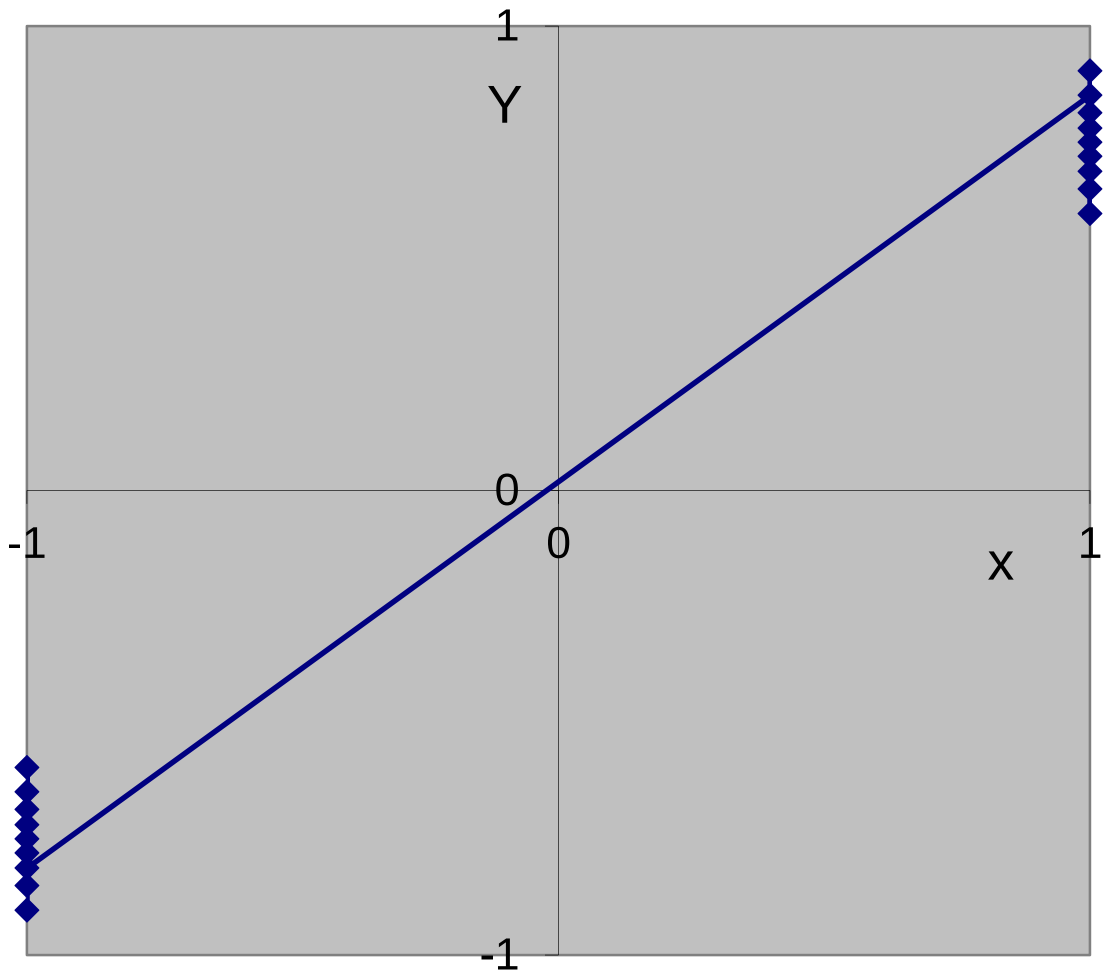
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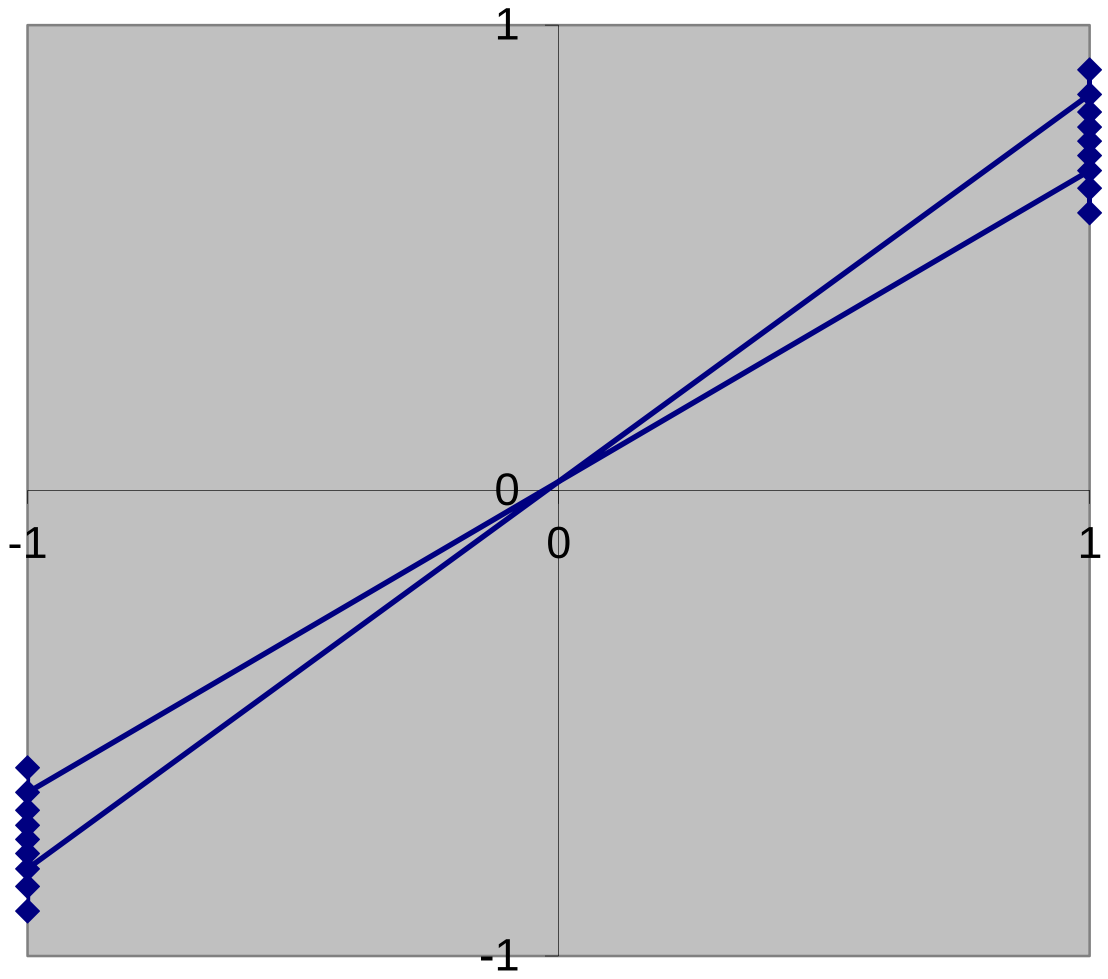
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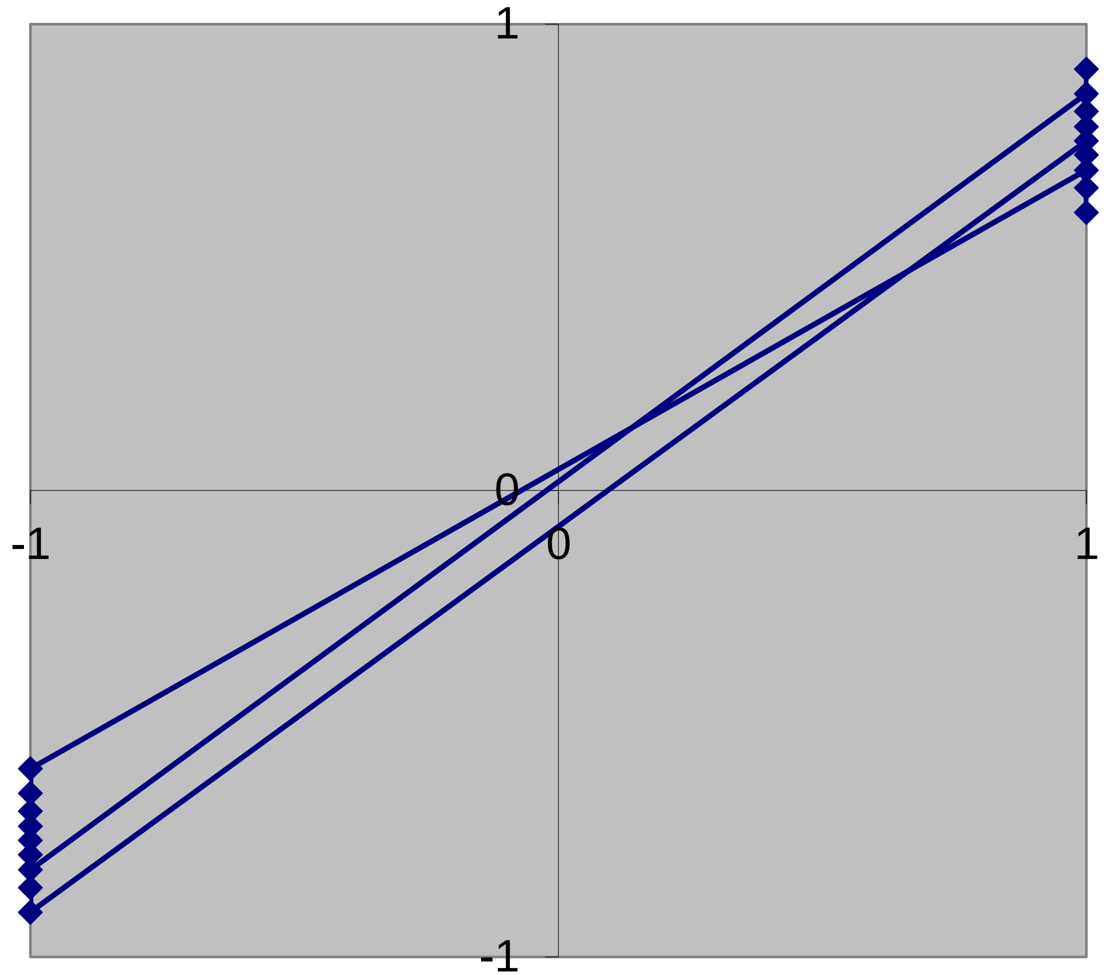
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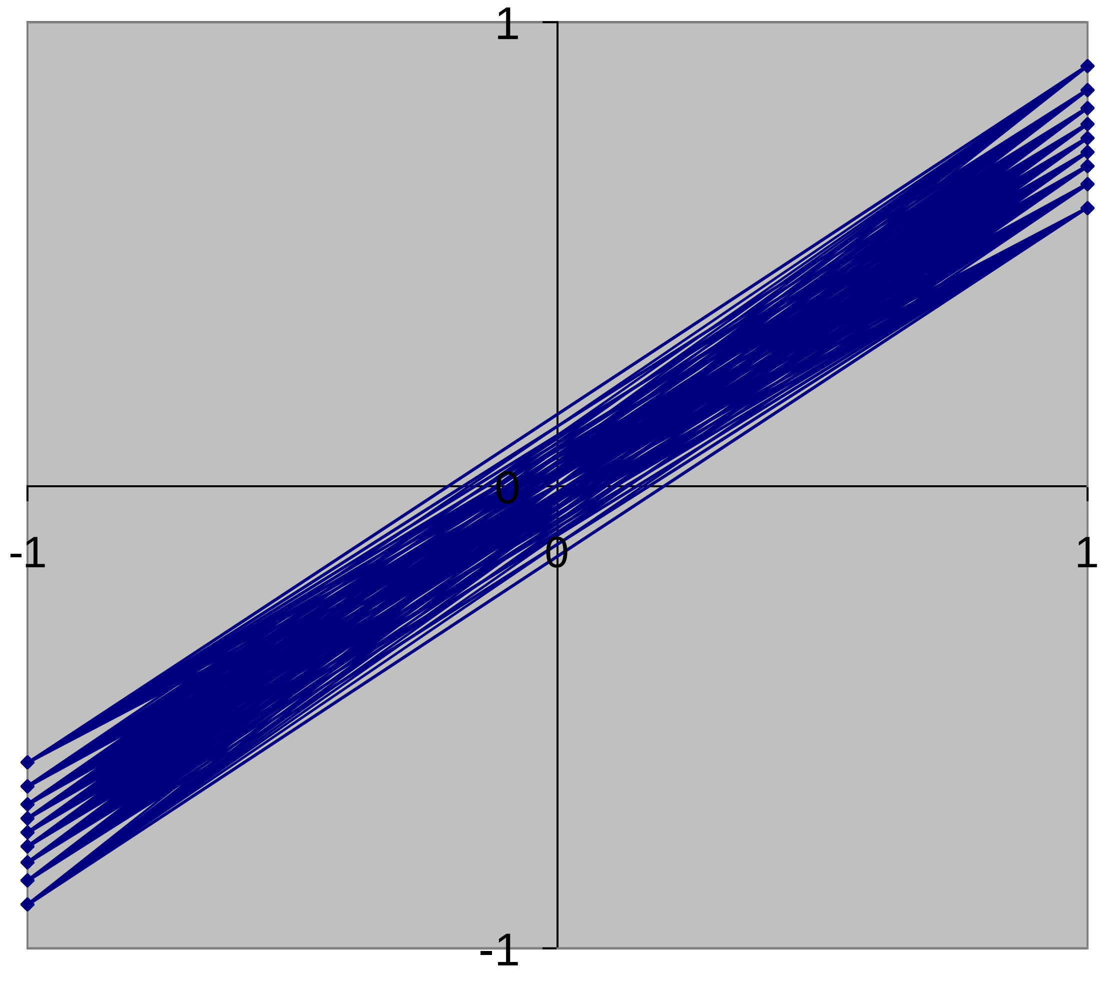
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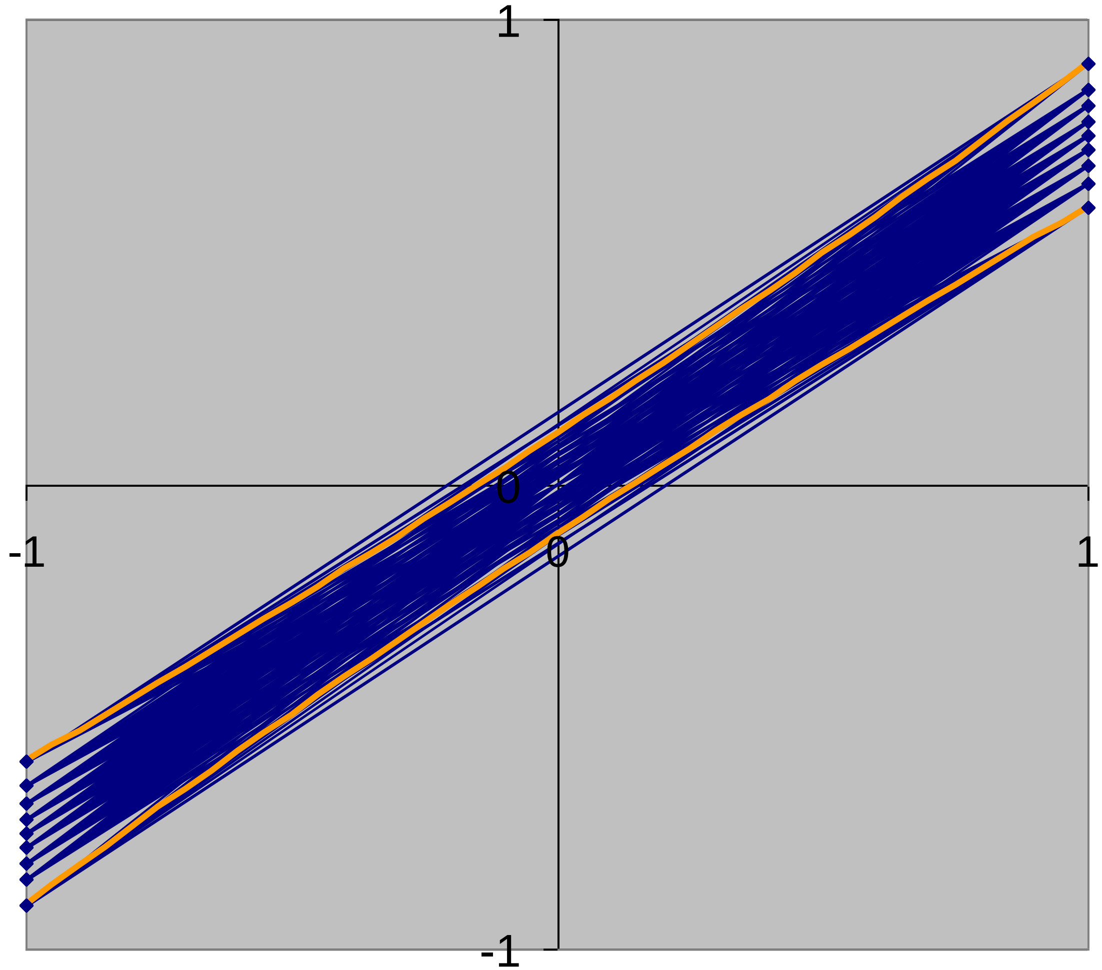
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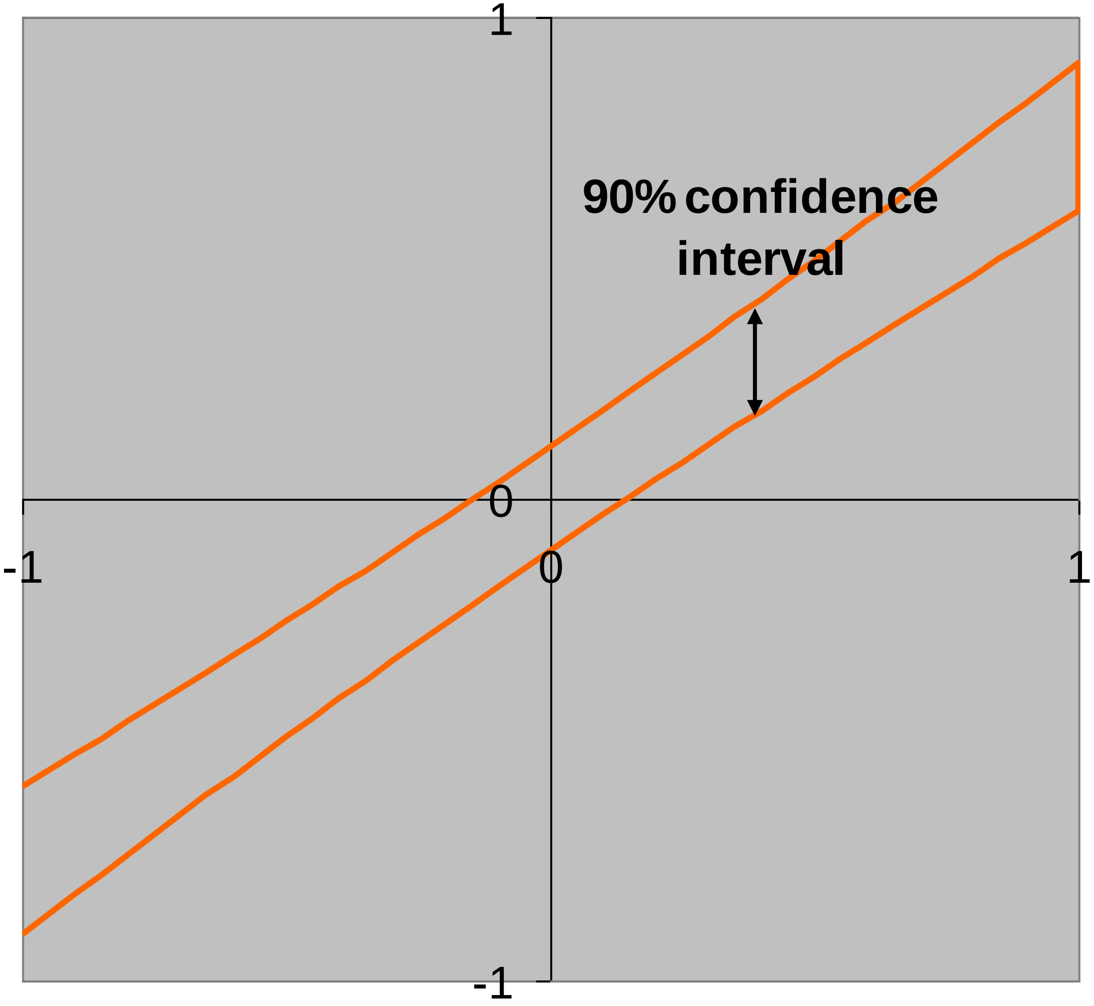
Surprise #1: Variance is less between data points*



*at least for this case

Surprise #2

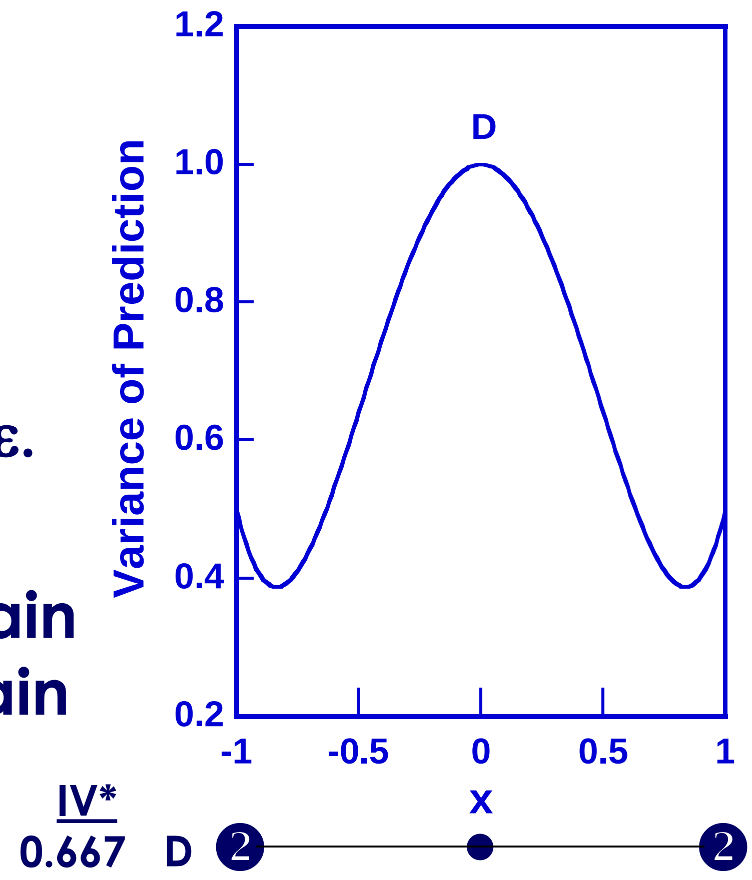
Example:

D-optimal design for fitting a parabola with N=5 points.

Model:

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_1^2 + \varepsilon.$$

Curie's symmetry principle*: When certain causes produce certain effects, the symmetry elements of the causes must be found in the effects.



***Lorsque certaines causes produisent certains effets, les éléments de symétrie des causes doivent se retrouver dans les effets produits.**

Surprise #2

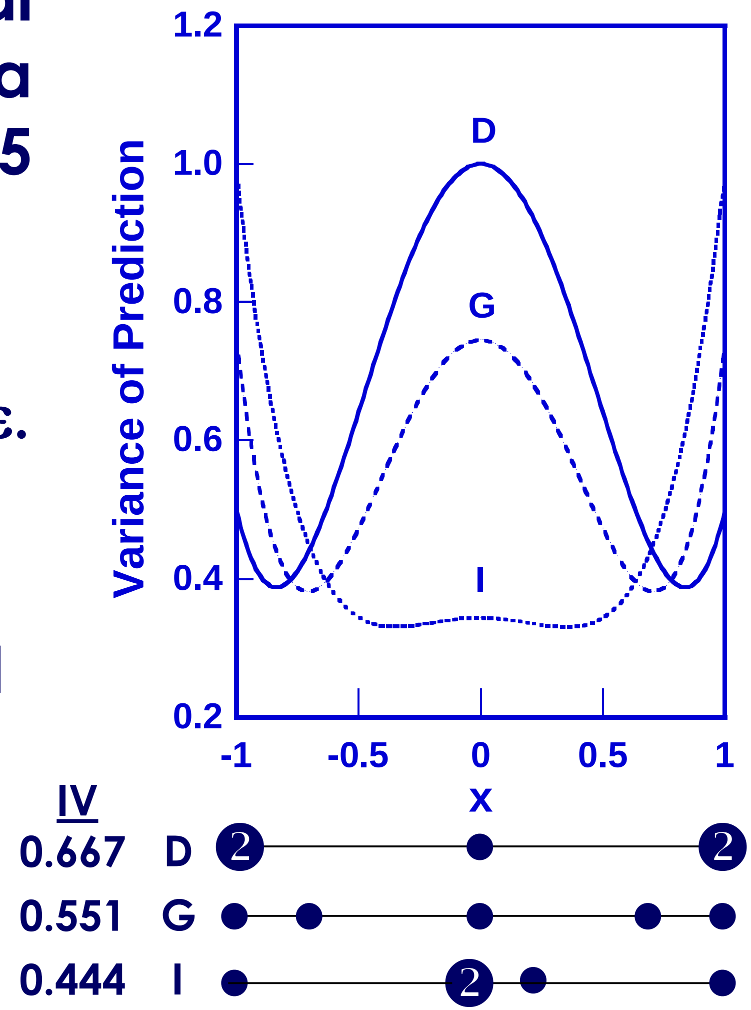
D-, G-, and I-optimal designs for fitting a parabola with N=5 points.

Model:

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_1^2 + \varepsilon.$$

Surprise: Despite Curie's principle, Optimal designs need <u>not</u> have the full symmetry of the problem statement.

Broken symmetry. →



Plot inspired by Fig. 3 of Linda Haines, The application of the annealing algorithm to the construction of exact optimal designs for linear–regression models, *Technometrics* **29** (4), pp. 439-447.

Digression: Integrated microsensor example

Research (Univ. of Michigan Center for Integrated Sensors & Circuits, c. 1989, with Wayne Baer, John Cowles, and Ken Wise) on integration of:

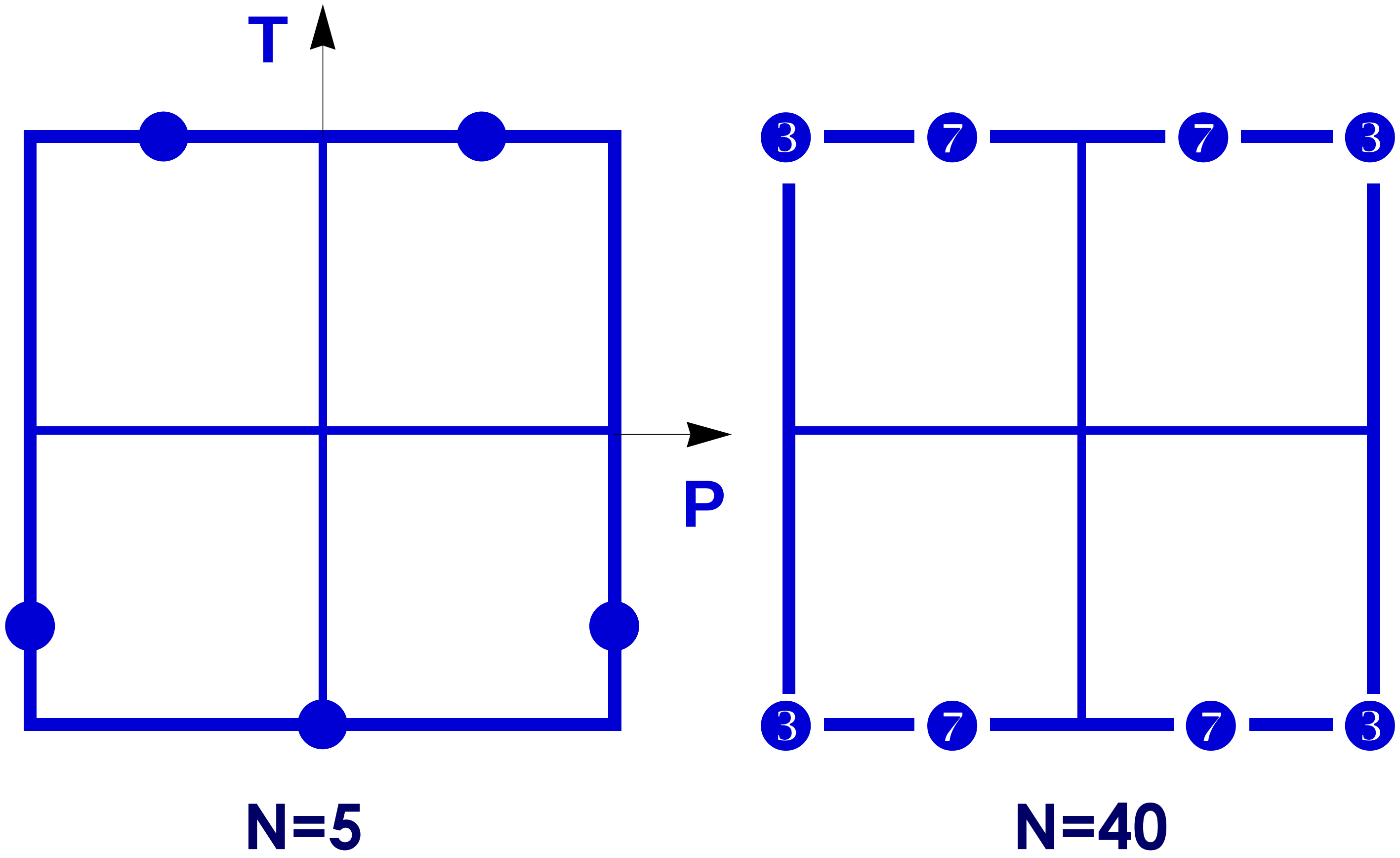
- Si-based, micromachined, capacitive (C) pressure (P) sensors
- thermometers (T)
- compensation circuits

Starting point: What's the function C=C(P,T)?

For each of several pressure sensors, large tables of C, P, and T were being generated, using a computer-controlled environmental chamber. Regression fitting. Independent definition of I-optimality.

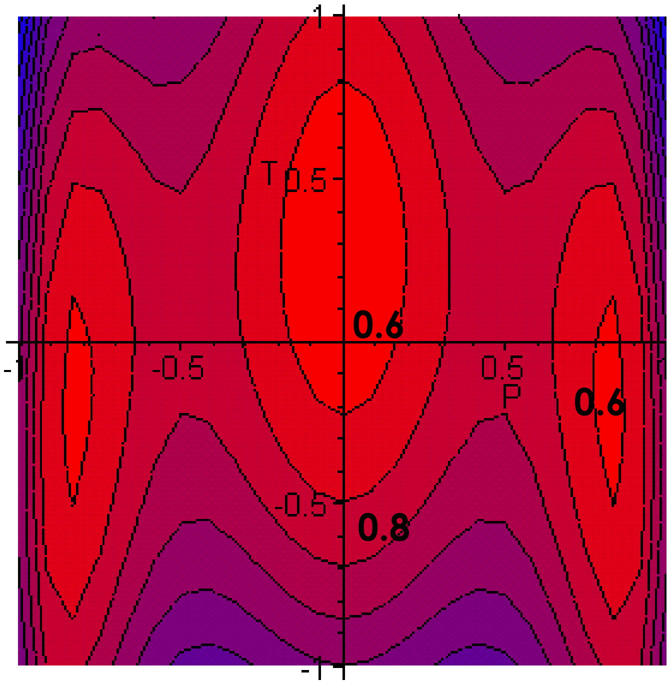
I-optimal Designs for

$$C(P,T) = \beta_0 + \beta_1 T + \beta_2 P + \beta_3 P^2 + \beta_4 P^3 + \varepsilon$$

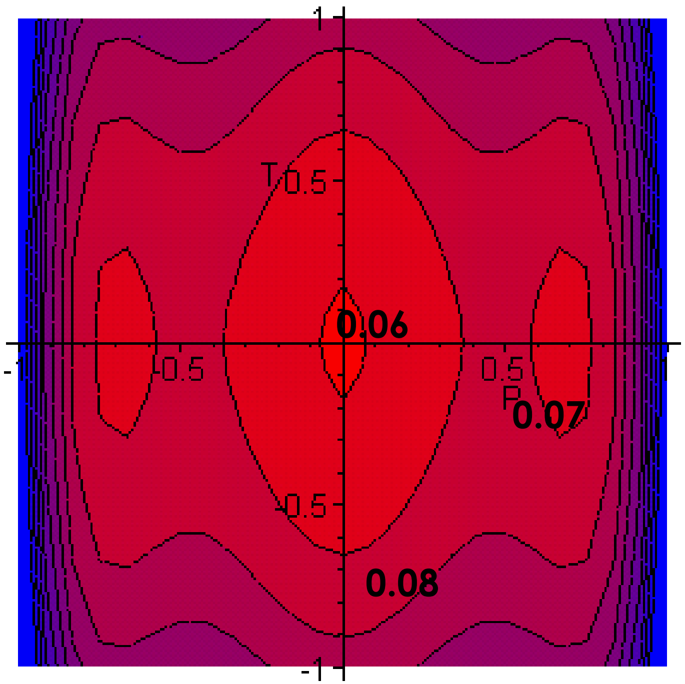


Variance Contours of I-optimal Designs for

$C(P,T) = \beta_0 + \beta_1 T + \beta_2 P + \beta_3 P^2 + \beta_4 P^3 + \varepsilon.$



N=5



N=40

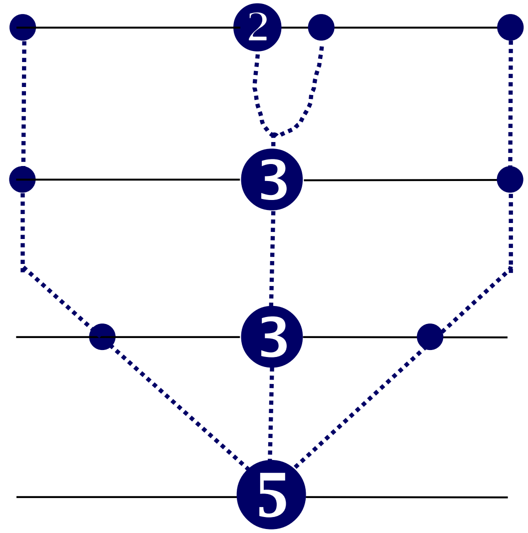
Surprise #3: Phase transitions in DOE

I-optimal design for fitting a parabola with N=5 points:

$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_1^2 + \varepsilon.$

The I-optimal design, with equal emphasis for prediction over x∊[-1,1], is →

As more emphasis is placed on prediction in the central region, the three central points shift inward, and merge into a single point, where three readings should be taken …



"Phase transitions"

Availability of free, optimal-design software

1991-2000: I-OPT

I-OPT was the first design of experiments system for finding I-optimal designs over continuous spaces. I-OPT was a derivative work (under a c. Y1989 agreement between the Univ. of Pietermaritzburg, S. Africa and the Univ. of Michigan, Ann Arbor) of Dr. Linda Haines' UNIVAC code with the same name. At the Univ. of Michigan, the code was converted to FORTRAN 77, extended and made available, via FTP, starting in Y1991, and via the World-Wide Web, starting in Y1996.

Ref: S.B. Crary, J.R. Clark, and K. Kuether, "I-OPT User's Manual," updated August 1999.

2000-2009: WebDOE™

WebDOE was announced at the Joint Statistical Meetings in Indianapolis in Aug. 2000, as a Web-based system for statistical design of experiments. It was the first major statistical software system available on the Internet and had 3300+ registered users, when it closed in Dec. 2009. See Slide 33 for a sampling of WebDOE capabilities.

Direction-Set Optimizer

Both I-OPT and WebDOE™ used a custom-built, multi-start, downhill optimizer, based on the **direction-set method** motivated by Fig. 10.5.1 (see next slide of this presentation), as well as outlined, in Numerical Recipes in Press et al.'s Chpt. 10, "Maximization and Minimization of Functions"[1]. It also drew inspiration came from Richard P. Brent's book[2]. The code was extended to multiple–precision arithmetic and was tested to 500 digits of precision.

Coetaneous with I-OPT was Hardin and Sloane's double-precision Gossett, which used a **pattern-matching method**.[3] Gossett was made available, for non-commercial purposes, and the authors made custom modifications to accommodate users with initially non-conforming operating sytems, e.g., IBM AIX. Designs found on Gossett and I-OPT always agreed to the precision used.

[1]W.H. Press, S. Teukolsky, W.T. Vetterling, B.P. Flannery, Numerical Recipes in Fortran 77: The art of scientific programming, Vol. 1 of Fortran Numerical Recipes, Cambridge Univ. Press (1997), URL: https://websites.pmc.ucsc.edu/~fnimmo/eart290c_17/NumericalRecipesinF77.pdf.

[2]Richard P. Brent, Algorithms for Minimization without Derivatives, Prentice-Hall (1973).

[3]R.H. Hardin and N.J.A. Sloane, "A New Approach to the Construction of Optimal Designs," J. Statist. Plann. Inference **37**, 339-369.

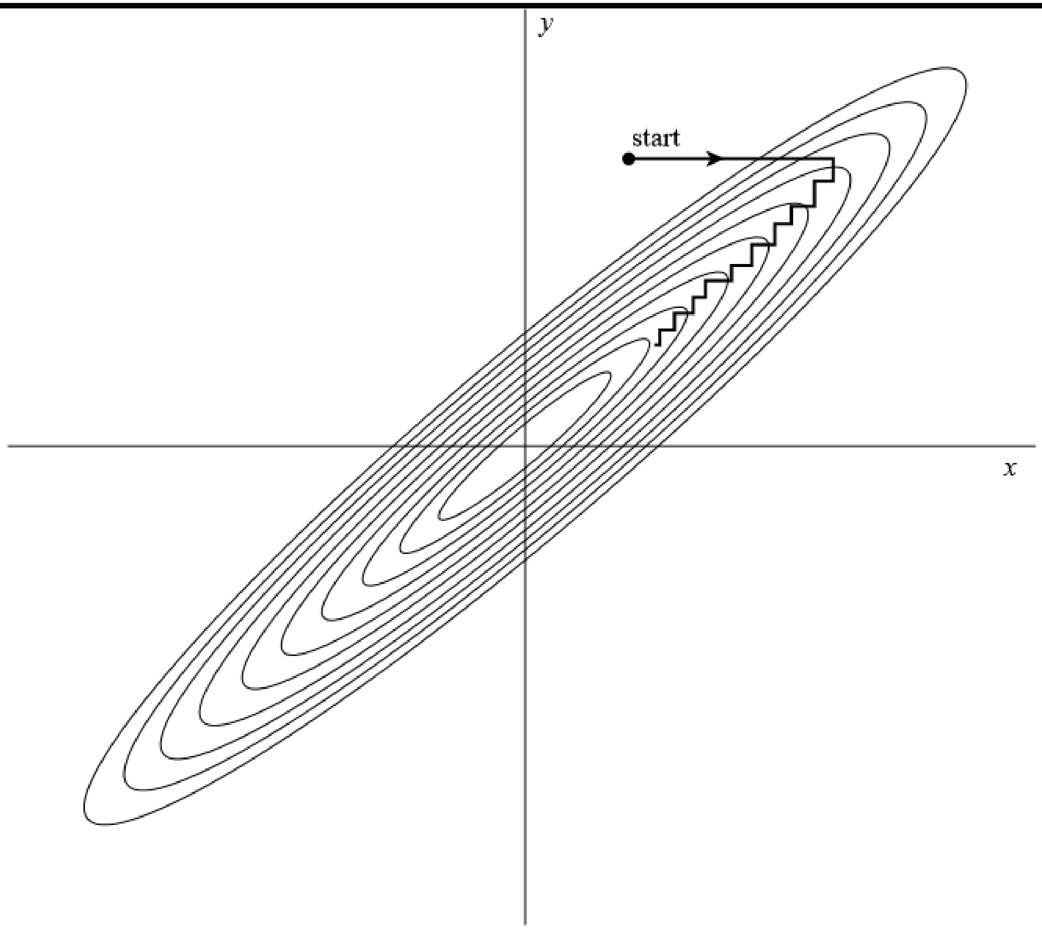


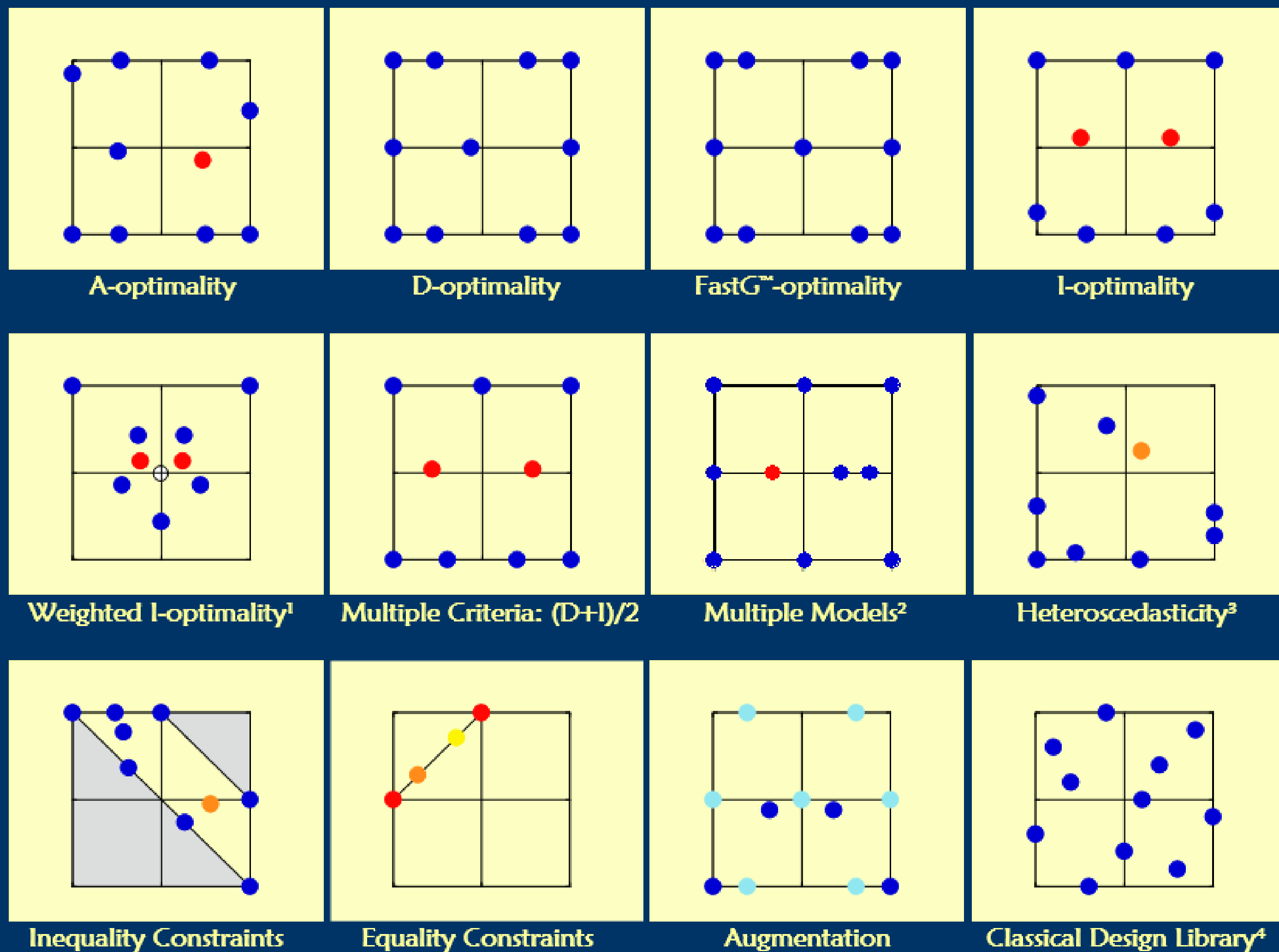
Figure 10.5.1. Successive minimizations along coordinate directions in a long, narrow “valley” (shown as contour lines). Unless the valley is optimally oriented, this method is extremely inefficient, taking many tiny steps to get to the minimum, crossing and re-crossing the principal axis.

Figure, above is from Press et al. reference, on the immediately preceeding page.

Direction-set methods allow line searches along non-Cartesian directions and thus allows for much more rapid convergence to the global minimum.

The Designs of WebDOE™

Aug. 2001 - Dec. 2009



Legend for last slide

For all[5] above designs, the model function is $Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2 + \beta_4 x_1^2 + \beta_5 x_2^2 + \beta_6 x_1^3 + \varepsilon$,

$\varepsilon \sim N(0,\sigma^2)$ (Note 6), i.i.d.; x_1 is horizontal and x_2 is vertical; 11 points

Notes:

[1] Weight falls off as origin-centered gaussian with std. dev. (0.1) given by the circle, thus placing maximum weight for prediction near the origin.

[2] Multiple Models: 0.9*IV(Full second-degree model) + 0.1*IV(Full second-degree model + x_1^3)

[3] Least error located at (-2,-2); error increases as inverse gaussian from that point.

[4] Uniform design

[5] Except multiple models: see Note 2.

[6] Except heteroscedasticity: see Note 3.

N.B.: In the above, all factors are quantitative. In practice, each factor may be quantitative, fixed-level, or qualitative.

3300+ registered WebDOE^{TM} users

DOE for physical experiments

15 years later:
I-optimality is the default objective function for response-surface methodology.

*DOE for *computer* experiments*

Definition of a computer experiment:

- Same input → same output (deterministic error)
- Something is known about how responses are correlated with distance between two sets of inputs.
- For the remainder of this presentation:

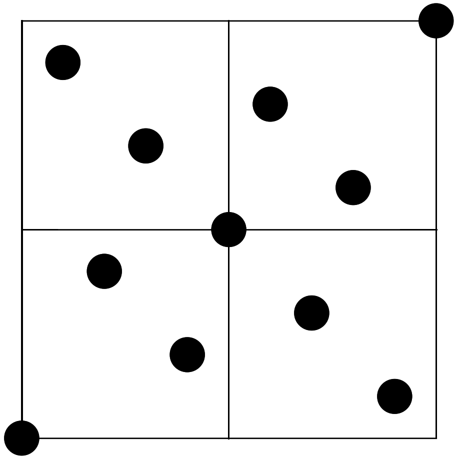
Model: $Y(x) = \beta_0 + Z(x)$

$cov[Z(s_1, s_2, \cdots, s_D), Z(t_1, t_2, \cdots, t_D)] = \sigma_Z^2 e^{-\prod_{d=1}^{D} \theta_d (s_d - t_d)^2}$

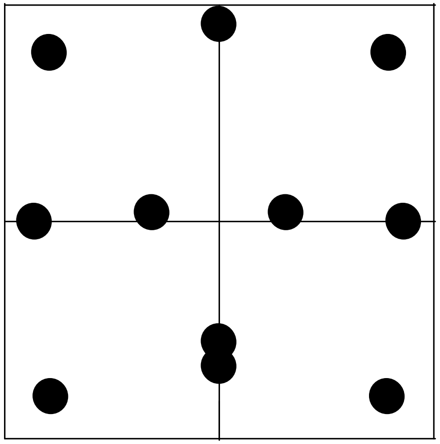
Assumed known θ's; N-point design ω_N; fit function $\hat{Y}(x)$

Objective: $\min_{\omega_N} \int_{-1}^{1} \int_{-1}^{1} E\{[\hat{Y}(x) - Y(x)]^2\} dx_1 dx_2 \cdots dx_D$

Surprise #4: Optimal twin-point designs



Latin hypercube design



IMSPE-optimal design with a twin point

Assumptions for the *N=11* IMSPE-optimal design:

Model: $Y(x) = \beta_0 + Z(x)$

$$cov[Z(s_1, s_2, \cdots, s_D), Z(t_1, t_2, \cdots, t_D)] = \sigma_Z^2 e^{-\prod_{d=1}^{D} \theta_d (s_d - t_d)^2}$$

$\theta_1 = 0.128,\ \theta_2 = 0.069$

Objective: $\min_{\omega_N} \int_{-1}^{1} \int_{-1}^{1} E\{[\hat{Y}(x) - Y(x)]^2\} dx_1 dx_2 \cdots dx_D$

Summary of Part 1: Surprises in DOE

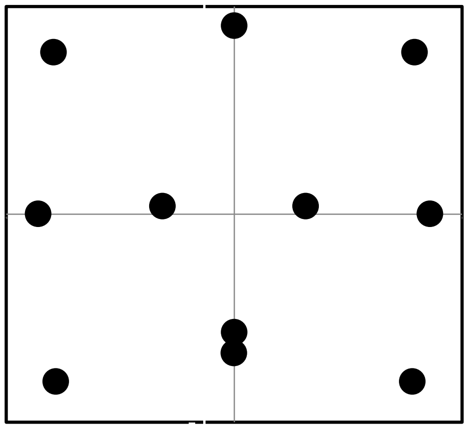
<u>for physical experiments</u>

1. Var of prediction can be less between loci of data.
2. Various optimality criteria and a violation of a naïve rule about symmetric causes → symmetric effects.
3. Phase transitions.

<u>for computer experiments</u>

4. Optimal twin-point designs ← focus of Part 2.

Part 2

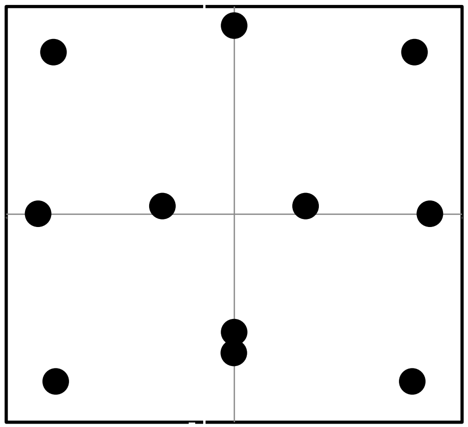


Woodcock IMSPE-optimal design with a twin-point, published 2002

"In any field, find the strangest thing and then explore it."

-- John Archibald Wheeler

Part 2



Woodcock IMSPE-optimal design with a twin-point, published 2002

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-- John Archibald Wheeler

Six objections to:

- the existence of optimal twin-point designs
- the use of twin-point designs in practice

Objections to twin-point designs

Objection #1

"Space-filling criteria ensure that the entire input space is sampled by preventing design points from being 'close' together."[1]

"Not only should the design points be spaced apart in the design space, …"[2]

"… making good predictions requires that inputs take many values over their range."[3]

[1]Erin Leatherman, Angela Dean, and Thomas Santner, Chapter 1, "Computer experiment designs via particle swarm optimization" (Jan 2014), URL: https://www.newton.ac.uk/files/preprints/ni14015.pdf.

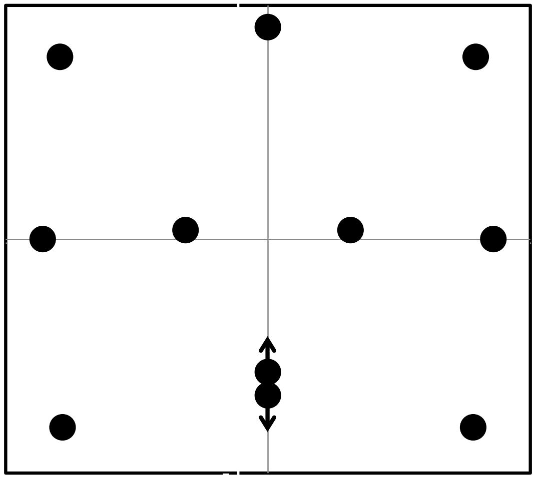
[2]Ryan Lekivetz and Bradley Jones, Fast flexible space-filling designs for non-rectangular regions, *Quality and Reliability Engineering International*, DOI: 10.1002/qre.1640 (2014).

[3]Ryan Lekivetz and Bradley Jones, Fast flexible space-filling designs with nominal factors for nonrectangular regions, *Quality and Reliability Engineering International*, DOI: 10.1002/qre.2429 (2018).

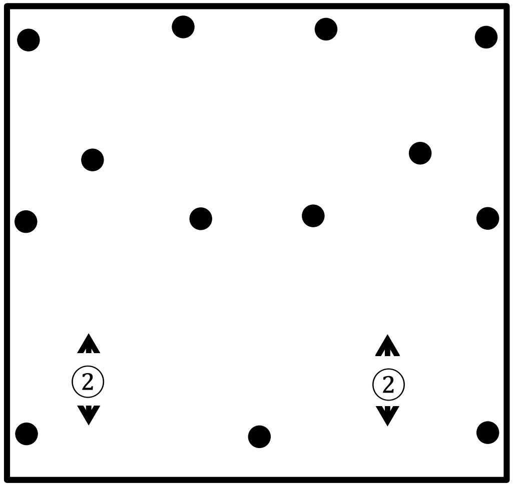
Objection #1

"Space-filling criteria ensure that the entire input space is sampled by preventing design points from being 'close' together." … …

Here are two counterfactual IMSPE-optimal designs:



Woodcock twin-point design
2002



Saunders duet-twin-point design
2019

Objection #1

"Space-filling criteria ensure that the entire input space is sampled by preventing design points from being 'close' together."

Non-sequitur statements, such as the above, are not just a problem in this corner of statistics. The following is a Jan 8, 2020 quote regarding the supposed requirement of "naturalness" in physics:

> "However, the particle-physics community has still not analyzed how it could possibly be that such a large group of people, for such a long time, based their research on an argument that was so obviously non-scientific. Something has seriously gone wrong here, and if we don't understand what, it could happen again."[1]

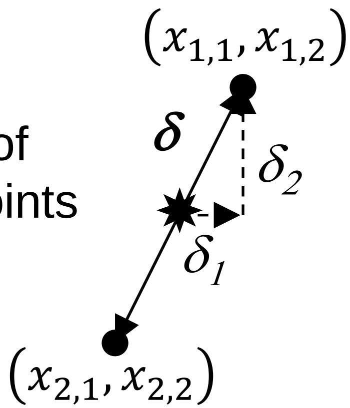
[1]Sabine Hossenfelder. "Physics update January 2020." *YouTube*, 8 Nov. 8, 2020, https://www.youtube.com/watch?v=yqokbIxDvIw, timestamp 4:45.

Objection #2

The IMSPE of twin-point designs cannot be computed, due to ill-conditioned matrices

$$IMSPE = 1 - trace\left(\boldsymbol{L}^{-1}\boldsymbol{R}\right)$$

A pair of twin points in D=2 factors



$$\boldsymbol{L} \equiv \left(\begin{array}{c|ccc} 0 & 1 & \cdots & 1 \\ \hline 1 & & & \\ \vdots & & \boldsymbol{V} & \\ 1 & & & \end{array}\right),$$

where $\boldsymbol{V_{i,j}} = e^{-\prod_{d=1}^{D}\theta_d\left(x_{i,d}-x_{j,d}\right)^2}$.

When there are two proximal points, $\boldsymbol{V}$ and $\boldsymbol{L}$ each has two ~equal rows, and thus each is highly ill-conditioned. If the twin points get close, the program for $\boldsymbol{L}^{-1}$ will fail. “NAN”

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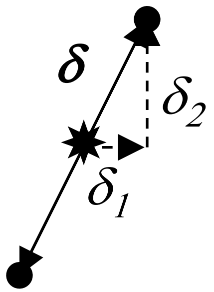
Solution: Use an extension of the Loh-Lam theorem[1] to avoid ill-conditioning of $\boldsymbol{L}$. Loh-Lam-C conjecture:



$$det(\boldsymbol{V}) = a\boldsymbol{\delta}^2 + b\boldsymbol{\delta}^4 + \cdots$$

$$det(\boldsymbol{L}) = A\boldsymbol{\delta}^2 + B\boldsymbol{\delta}^4 + \cdots$$

$$IMSPE = IMSPE_0 + \alpha\boldsymbol{\delta}^2 + \beta\boldsymbol{\delta}^4 + \cdots$$

[1]Wei-Liem Loh and Tao-Kai Lam, “Estimating structured correlation matrices in smooth gaussian random field models,” *Annals of Statistics* **28** (3), pp. 880-904 (2000).

Objection #3

Computationally intensive integrals in matrix $\boldsymbol{R}$

$$\boldsymbol{IMSPE = 1 - trace\left(L^{-1}R\right)}$$

$\boldsymbol{R}$ has elements with integrals like $\int_{-x}^{x} e^{-t^2} dt$ that are "… generally evaluated by a discrete sum over a finite grid …"[1]

[1]Luc Pronzato & Werner G. Müller, Design of computer experiments: space filling and beyond, *Stat. Comput.* **22**, pp. 681-701 (2012). Quote is from p. 690, Col. 2, ¶ 2.

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Computationally intensive integrals in matrix $\boldsymbol{R}$

$$\boldsymbol{IMSPE = 1 - trace\left(L^{-1}R\right)}$$

$\boldsymbol{R}$ has elements with integrals like $\int_{-x}^{x} e^{-t^2} dt$ that are "… generally evaluated by a discrete sum over a finite grid …"[1]

Solution: $\int_{-x}^{x} e^{-t^2} dt \equiv \sqrt{\pi}\, erf(x)$, where $erf(x)$ is the special function known as the "error function," which can be evaluated rapidly to effectively arbitrary accuracy (more than one-million digits, if required).

[1] L. Pronzato & W.G. Muller, Design of computer experiments: space filling and beyond, *Stat. Comput.* **22**, pp. 681-701 (2012). Quote is from p. 690, Col. 2, ¶ 2.

Objection #4

Design-point repulsion

“Effective attraction requires an explicit pair-wise attraction somewhere in the system.” --Nobel laureate, physics

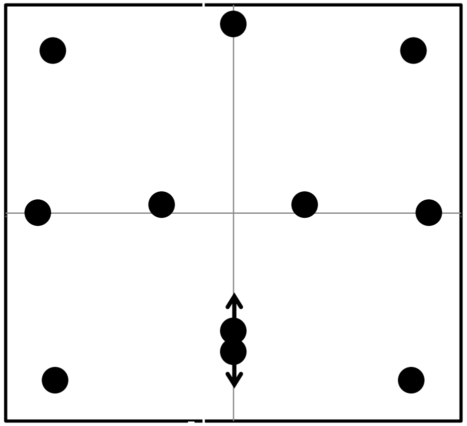
“… accounting for repulsion between points and thus favorising maximin-distance designs.”[1]

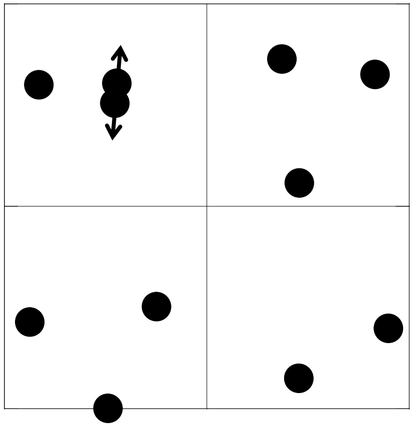
[1]Pronzato & Müller, op. cit., p. 696, Col. 2, ¶ 1.

Objection #4: *Design-point repulsion*

"Effective attraction requires an explicit pair-wise attraction somewhere in the system." --Nobel laureate, physics …

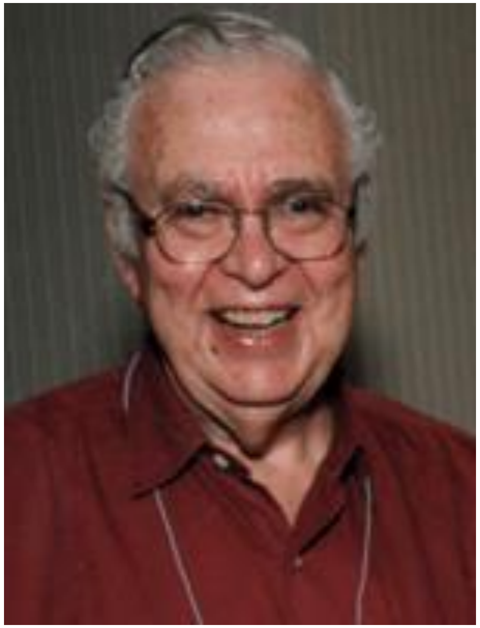
Counterfact: "The arranged marriage." The twin points are pushed together by the collective repulsion from others in the community. This repulsion grows ~proportional to the interpoint separations r_{ij}, $1 \le i, j \le N$ (in distinction to, e.g., r_{ij}^{-2} Coulombic repulsion), as well as by repulsion of each point from the boundary.





Objection #5

(Gene) Golub (1932-2007): “If you need more than double-precision, you don’t know what you’re doing.”



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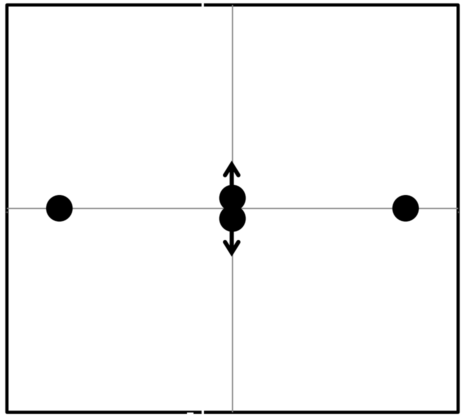
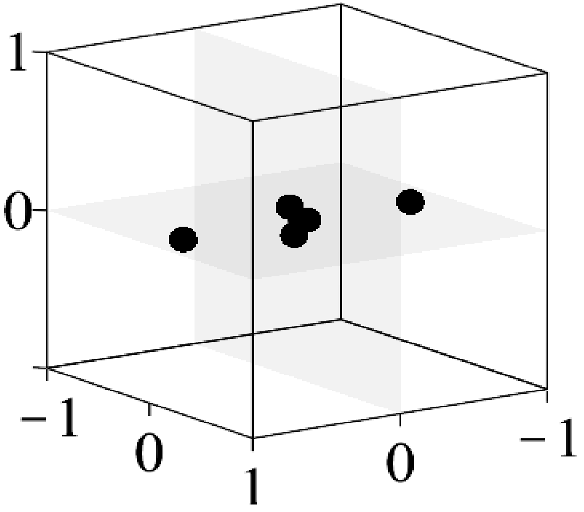
(Gene) Golub (1932-2007): “If you need more than double-precision, you don’t know what you’re doing.”

C, at first: Golub’s rule is <u>no longer</u> valid. Modern science and technology will increasingly require quadruple- (and higher-) precision arithmetic.



Stormann twin-point design
2015



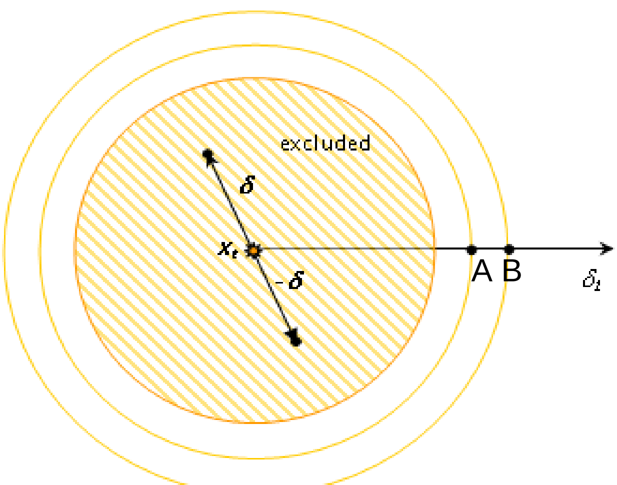
Saunders triplet-point design
2019

Both: FORTRAN, with ~32 digits

Objection #5

(Gene) Golub (1932-2007): “If you need more than double-precision, you don’t know what you’re doing.”

C, now: Wait a minute! Maybe there <u>is</u> a way to find twin-point designs using only double-precision arithmetic.



There is severe ill-conditioning, when *d* < *10* $^{-6}$, but the form of the *IMSPE is known, viz.,*

$$\lim_{\substack{\delta_2=0 \\ \delta_1\to 0}} IMSPE/\sigma_Z = a_0 + a_1\delta_1^2 + \cdots ,$$

so, fit and extrapolate.

Design-point label	δ_1	$x=\delta_1^2$	$IMSE/\sigma_z^2$
A	0.00120	0.0000144	0.7460920868…
B	0.00140	0.0000196	0.7460912887…
x_t via extrapolation	0	0	0.7460942972…
x_t via symbolic analysis	0	0	0.7460942972…

This “quasi-holographic continuation” solves the problem.

Objection #6

If twins *fully merge*, then an intractable singularity appears.

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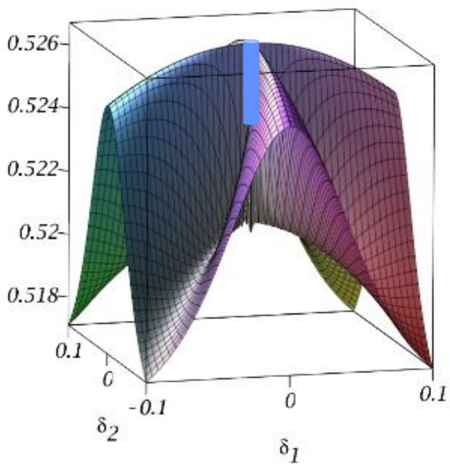
If twins *fully merge*, then a singularity appears.

Solution: Generalize IMSPE. Then, expand it and its “post” (shown in blue, below) into singular and non-singular parts.



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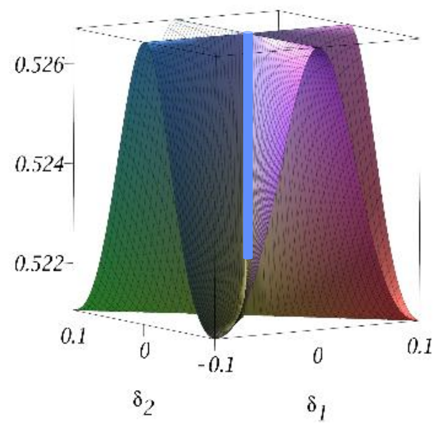

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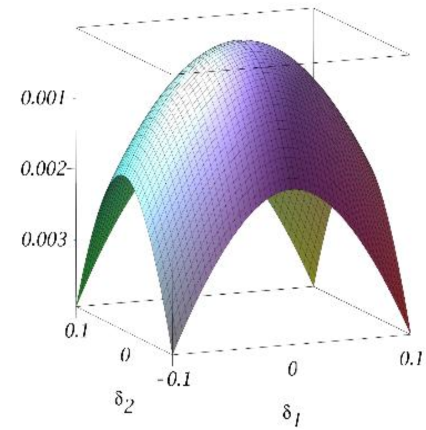

$$IMSPE = IMSPE_{singular} + IMSPE_{non-singular}$$

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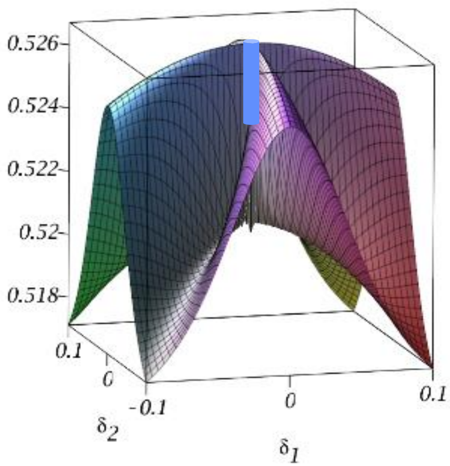

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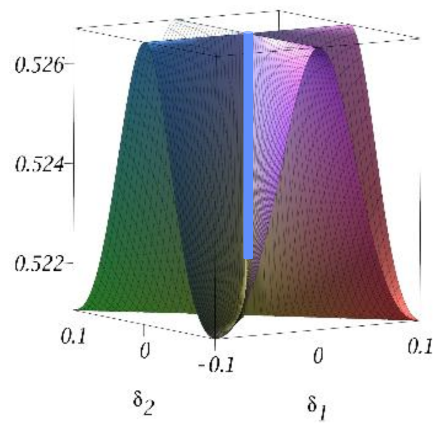
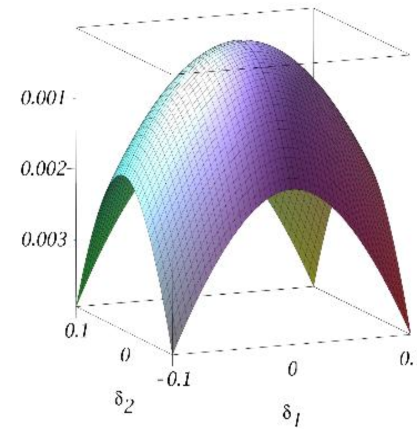


$+$



$$IMSPE = IMSPE_{singular} + IMSPE_{non-singular}$$

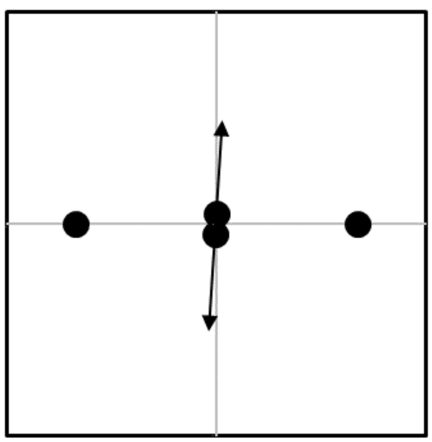
$IMSPE_{singular}(\varphi)$ has a continuous, extra dimension φ.

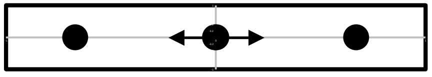
Do difficult singularities and extra dimensions sound familiar? Higher-dimensional posts can exist as sheets or “branes.”

For Q&A: One more objection

Objection #7 Designs with proximal points have poor projective properties.

Solution for a typical case: If a pair of twin points is oriented along a spatial direction that might subsequently be determined to be irrelevant, then rotate the twins about a normal to its center by a very small angle. If the spatial direction proves to be irrelevant, the projected design will still have a tractable twin. In general, if one abandons one's prejudice against twins, then, with a modicum of care, projected twins can remain twins.





Part 3

Some *very serious* speculation

Think the Unthinkable

"Why String Theory is Right"[1]

"Let's actually start with the regular old point particles of The Standard Model. When a point particle is moving through space and time it traces a line. On a spacetime diagram, time versus one dimension of space, this is called its world line."

[1]PBS Great Courses Plus. "Why String Theory is Right." *YouTube*, 7 Nov. 2018, https://www.youtube.com/watch?v=iTTa9YcTe1k.

Think the Unthinkable

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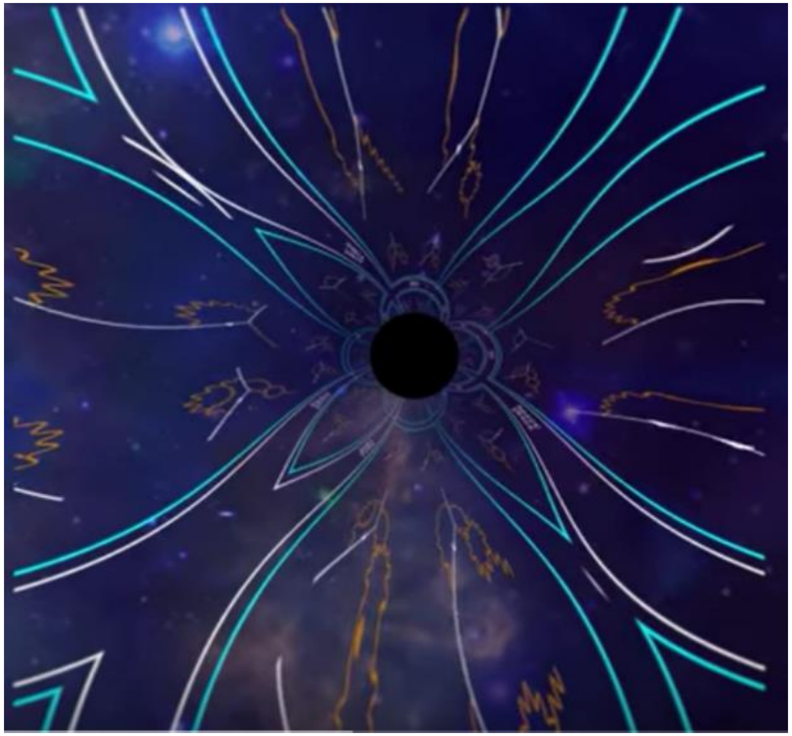
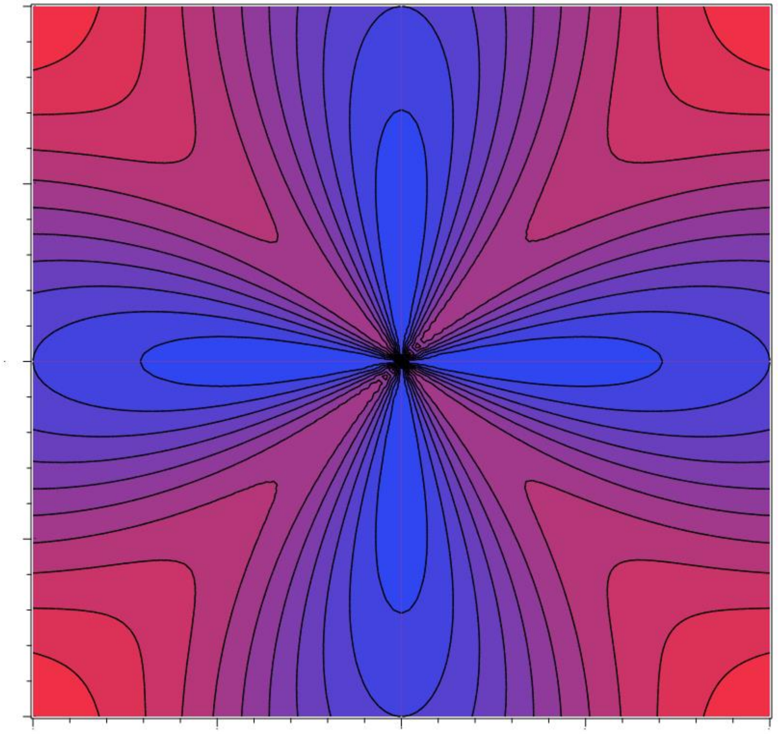
Think the Unthinkable



“Why String Theory is Right,” 4:21. Due to the singularity at the center, a disk is excluded in string theory.



IMSPE: 3 evenly spaced points. The singularity at the center is treated with integrable Nu math.

Can DOE & quantum field theory learn from each other?

<u>DOE for computer experiments</u>

Points represent trials.

Twins, triplets, …, m-uplets.

Objective function can be cast in Hamilton's-principle form:

$\min_{\omega_N} \int MSPE\, \boldsymbol{dx}$.

Needs a dynamical, relativistic IMSPE generalization.

Has singularities in the form of essential discontinuities.

Integrable (exact solution).

Rational polynomials are vital.

Information-theory approach.

Nu-class low-degree-truncated rational generalized functions.

~70% of points are singletons, with repulsion proportional to r.

<u>Quantum field theory</u>

Points represent particles.

2 or more particles interact.

Hamilton's principle:

$\delta \int_{t_1}^{t_1} \mathcal{L}(q_i, \dot{q}_i, t)\, dt = 0$,

where $\mathcal{L}$ is the Lagrangian.

Is dynamic and relativistic.

Has problematic singularities.

Non-integrable, presently.

Rational polynomials are important.

Info.-thry approaches under study.

Calabi-Yau manifolds.

~70% of energy is dark energy, with repulsion proportional to r.

Can DOE & string theory learn from each other?

Roger Penrose, Prof. of Mathematics (emeritus) at Oxford Univ. has the following two principal objections to string theory:[1]

- The requirement for compactified extra dimensions.
- Function proliferation: There are ~10^{500} ways (or possibly an infinite number of ways) the extra dimensions can be geometrized.

DOE, in its realm, answers these objections, as follows:

- Non-compactified extra dimensions are introduced naturally, via generalized functions.
- By an extension of the Loh-Lam conjecture, the action must be in the restrictive class of low-degree-truncated, rational, generalized functions. (see papers on arXiv.org and Authorea.com.)

In addition:

- Nu math allows for the singularities to extend over the entire geometric space, thus allowing for non-locality.
- A background-independent theory may be possible.

[1]Roger Penrose, Fashion, faith, and fantasy in the new physics of the universe, Princeton Univ. Press (2016).

Q&A

Q (Charles Chen): *In the integrated microsensor example, is the MSPE roughly constant in the central region of the prediction domain, as it was for the simple parabola example of Slide #25?*

A: Yes, as you can see on Slide #28, the MSPE is relatively constant over the central region of the prediction domain, in comparison to the IMSPE near boundary of the domain, especially near the extreme ends of P.

Q (Don Mintz): *How reliable is the existence of twins?*

A: This is an excellent question, given the ASQ Statistics and Reliability Discussion Group's obviously strong interest in reliability. It would be an appeal-to-authority fallacy to accept the existence of IMSPE-optimal twin-point designs, just because the speaker claims they exist; just as it would be a fallacy to accept the view that IMSPE-optimal designs are impossible, based on one or more of the objections discussed in this talk.

I can tell you this: We have checked, and always accepted as true, the **theoretical** IMSPE given in linear-algebra form as Eq. 2.9 of the Y1989 paper by Sacks, Schiller, and Welch (SSW).

SSW's Eq. 2.9 has been evaluated **numerically** and compared to competing designs, by members of the author's group (a high-schooler, undergraduates, graduate students, a systems programmer, a mathematics professor at the U. of Vienna, a start-up entrepreneur, an engineer with a day job in a high-tech industry, and a Stanford research professor) using FORTRAN, Excel, and Maple programs; running on DOS, Unix, IBM AIX, Linux, and various Apple operating systems; using double-, quadruple-, and up-to-500-digit extended-precision arithmetic. Independently, SAS/JMP provided an alternative evaluation. The limit of the IMSPE, as the separation between two twin poiints goes to zero, has been shown to be parabolic (Crary, 2016), and this has always agreed, to the precision in use, with numerical studies. In short, all comparisons of numerical evaluations have agreed with SSW's Eq. 2.9.

We have never faced the conflict about which Hermann Weyl wrote, "My work always tried to unite the true with the beautiful, but when I had to choose one or the other, I usually chose the beautiful," because IMSPE-optimal twin-point designs, by their nature, carry both attributes - truth and beauty - without diminution of one by the other.

References for DOE, with emphasis on computer experiments

Through Y2002, see the reference at the bottom of Slide 34.

Since Y2002, see the following books. Nota bene: None mentions twin-point designs.

Angela Dean, Daniel Voss, and Danel Draguljić, Design and analysis of experiments, 2nd ed., Springer (2017). This has a new chapter on computer experiments.

Thomas J. Santner, Brian J. Williams, and William I. Notz, The Design and Analysis of Computer Experiments, Springer (2018).

Handbook of design and analysis of experiments, edited by Angela Dean, Max Morris, John Stufken, and Derek Bingham, CRC Press, Taylor & Francis Group, LLC, (2015). This has an introduction to linear models by Linda Haines, as well as four chapters devoted to computer experiments.

Bradley Jones and Douglas C. Montgomery, Design of experiments: a modern approach, Wiley (2019).

Peer-reviewed paper on twin-point designs: SC, "Design of Computer Experiments for Metamodel Generation," *Special Invited Issue of Analog Integrated Circuits and Signal Processing* **32**, pp. 7-16 (2002). A version with minor corrections is available at the author's blog,

SC's recent papers on twin-point designs in computer experiments, co-authored with various collaborators and including references to earlier research, are available on his blog, as well as at the following arXiv.org and Authorea.com URL's:

https://arxiv.org/search/?query=Selden+Crary&searchtype=all&source=header (six papers).

https://www.authorea.com/users/270307/ (two Y2019 papers).