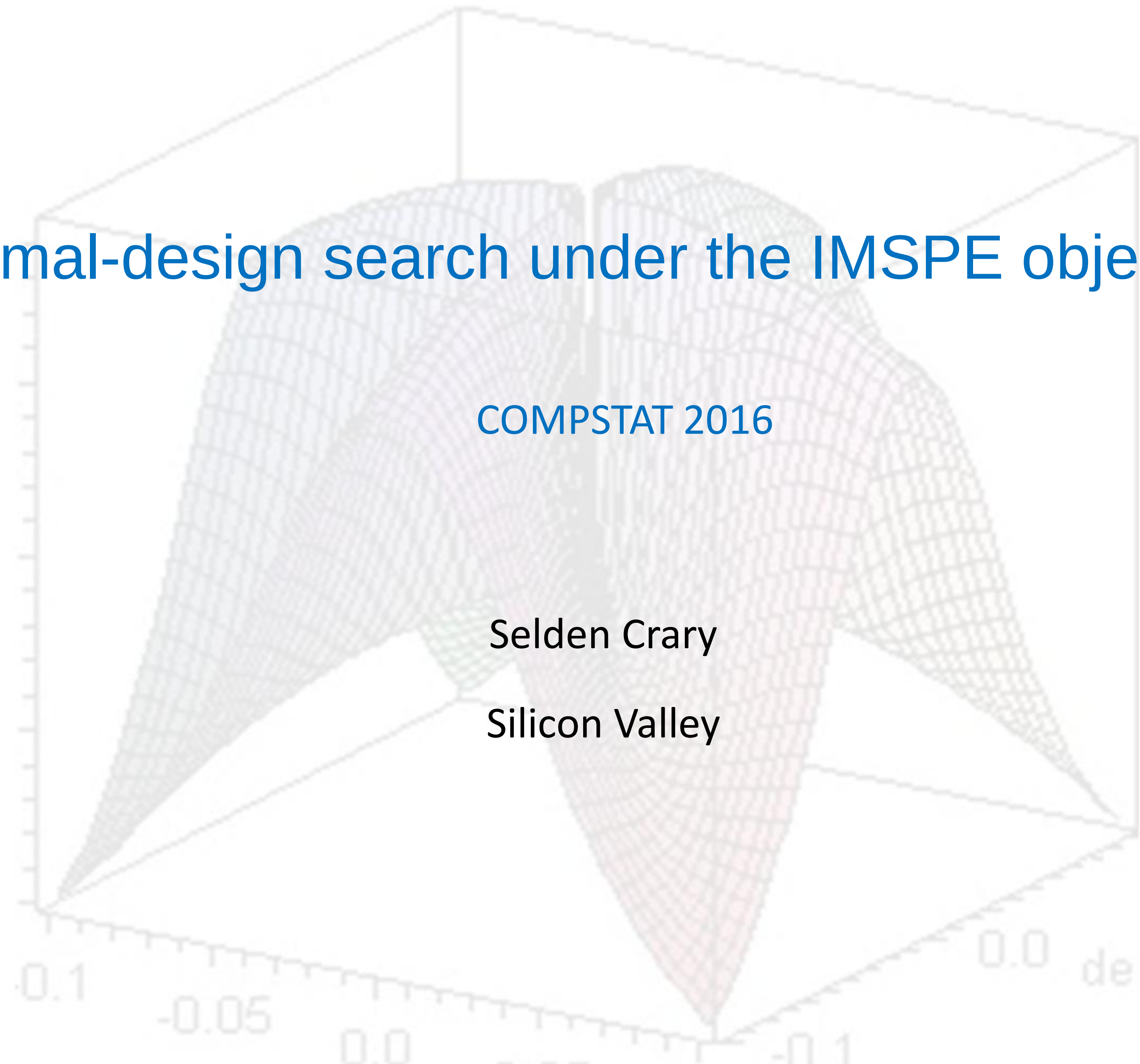


Optimal-design search under the IMSPE objective

COMPSTAT 2016

Selden Crary

Silicon Valley

Outline:

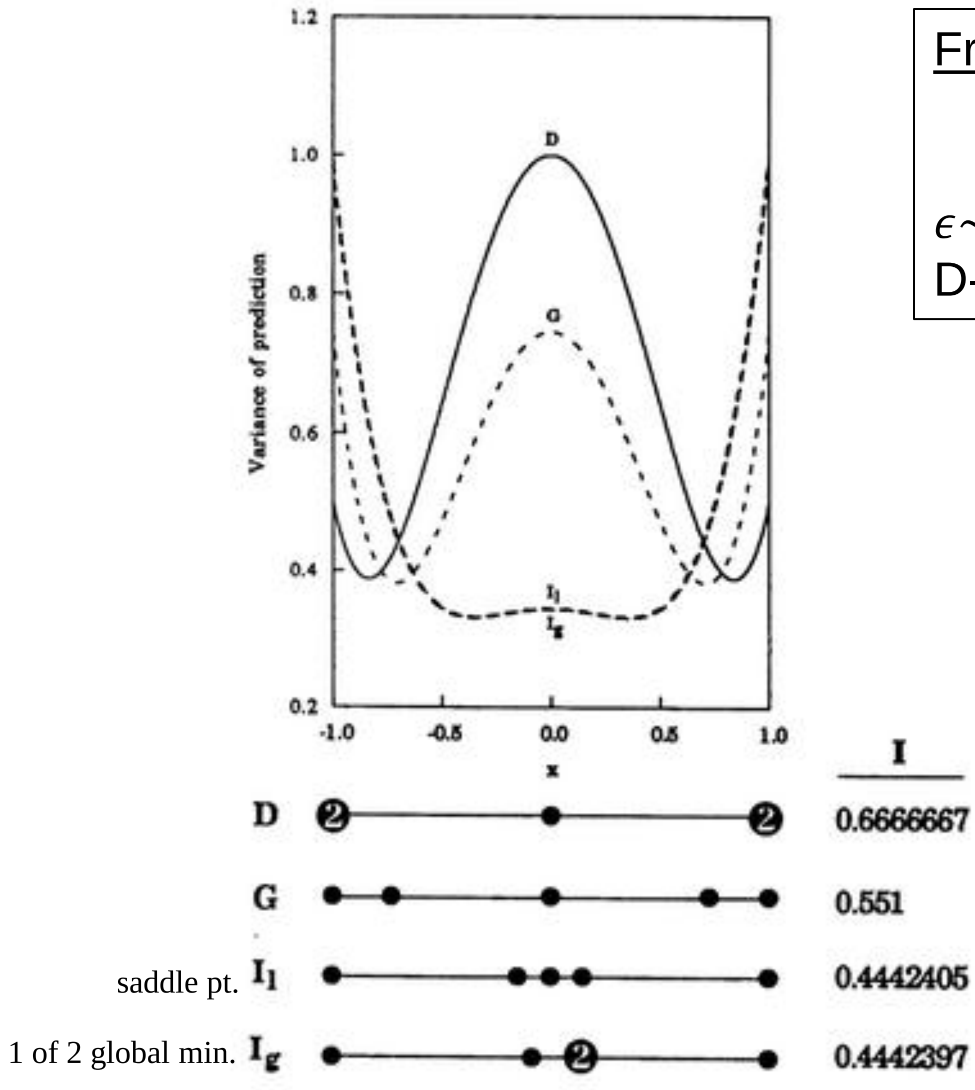
1. 1D designs for physical exp'ts: COMPSTAT 1992
2. 2D designs for computer exp'ts with "twin-points"
   a) N=4
   b) N=11
   c) Phase diagram of water
3. "Nu class" of low-degree-truncated rational functions
   a) Active theory
   b) Conjectures & Mild-to-wild speculations
   c) Parting thought, invitation, contacts, other active collaborators, collaboration space
   d) qMinos+X from Stanford Univ.

From COMPSTAT 1992 book*

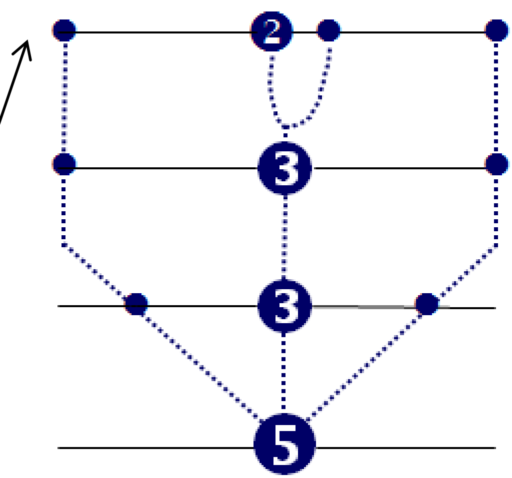
$$Y = \beta_0 + \beta_1 x + \beta_2 x^2 + \epsilon$$

$\epsilon \sim N(0, \sigma_Z{}^2), N = 5$

D-, G-, and I-optimal designs



Ig–optimal designs for differently weighted integrals



*Crary, Hoo, & Tennenhouse

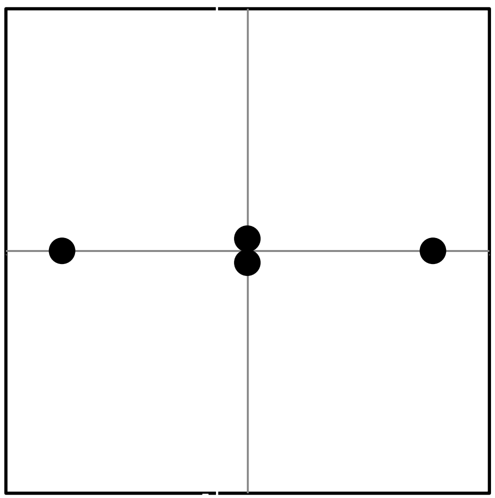
From Crary & Stormann arXiv paper, 2015

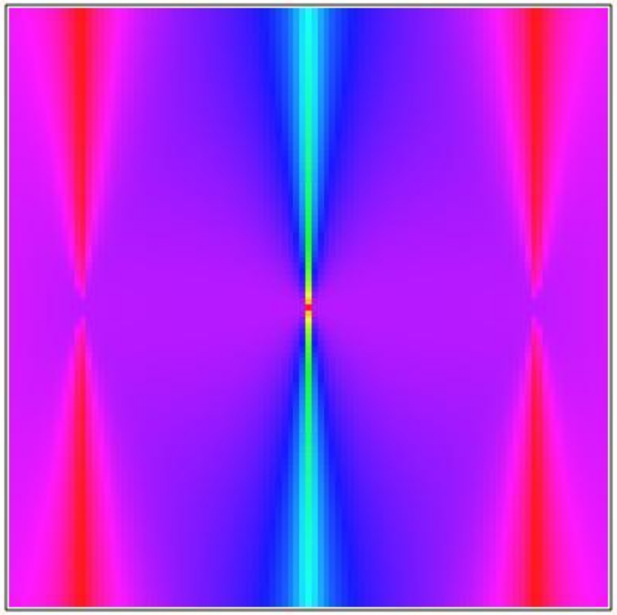
Usual Gaussian-process model

Gaussian covariance matrix: $\boldsymbol{V}_{i,j} = exp\left[-\theta_1\left(x_{i,1} - x_{j,1}\right)^2 - \theta_2\left(x_{i,2} - x_{j,2}\right)^2\right]$

Response: $Y(x_1, x_2) = \beta_0 + Z,$ à $la\ Sacks, Schiller, \&\ Welch$ 1989; $N = 4$

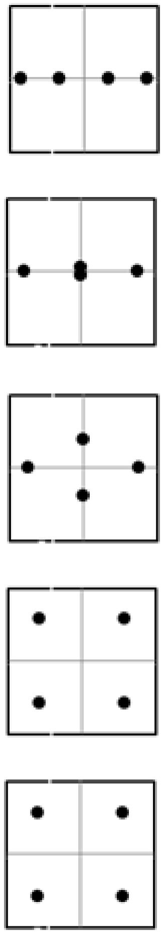
IMSPE-optimal designs: $\min_{\omega_N} \int E\left[\left(\hat{Y} - Y\right)^2\right] \boldsymbol{dx}$

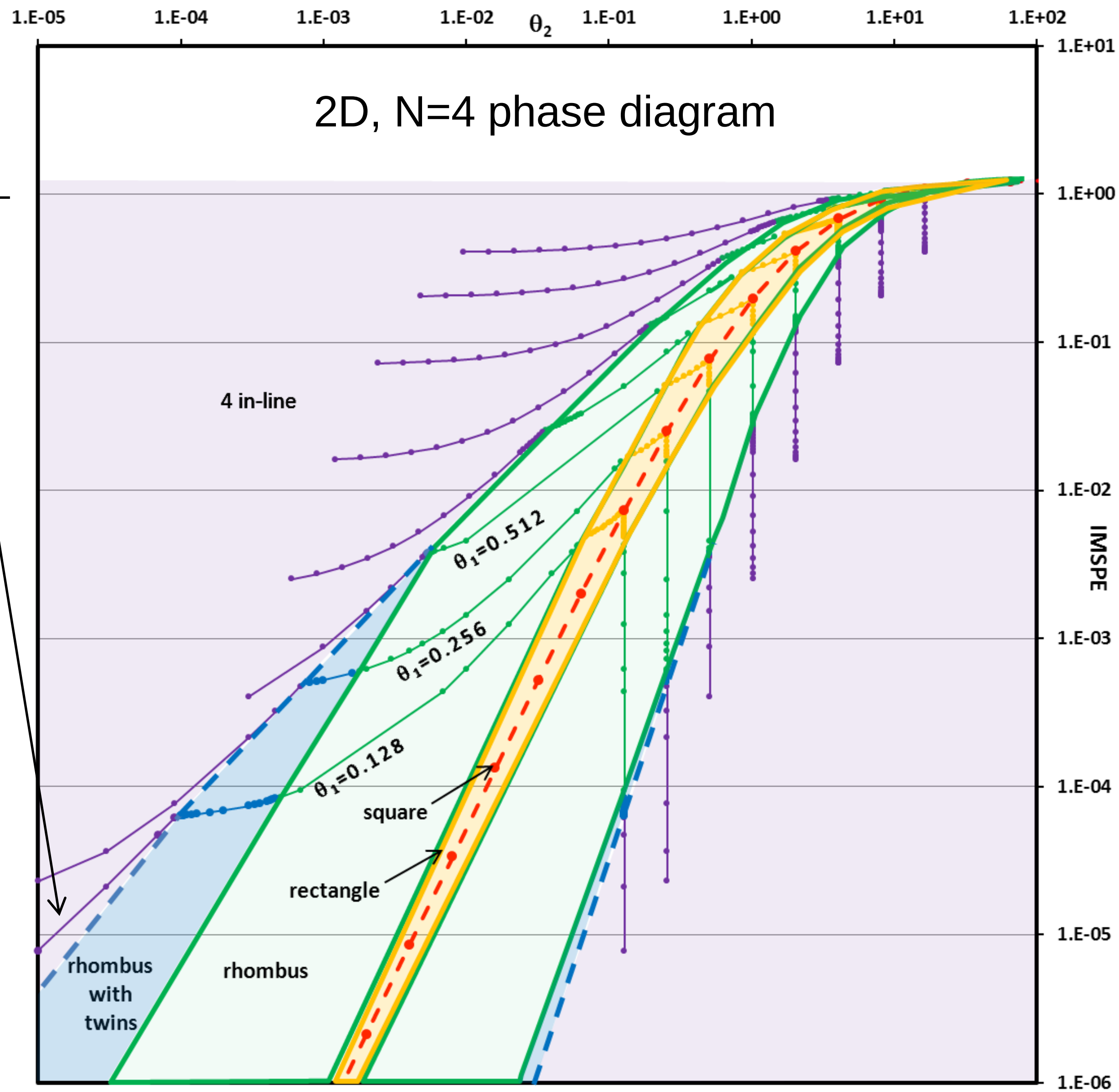




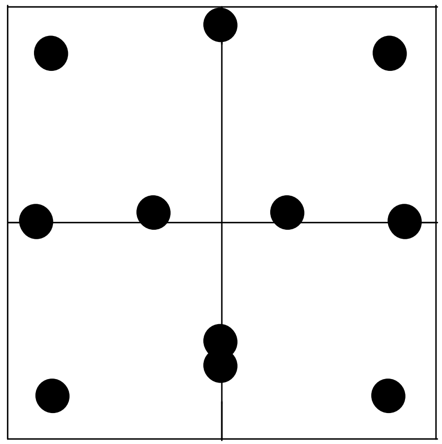
Rainbow plot of IMSPE

Phases along
$\theta_1 = 0.128$:

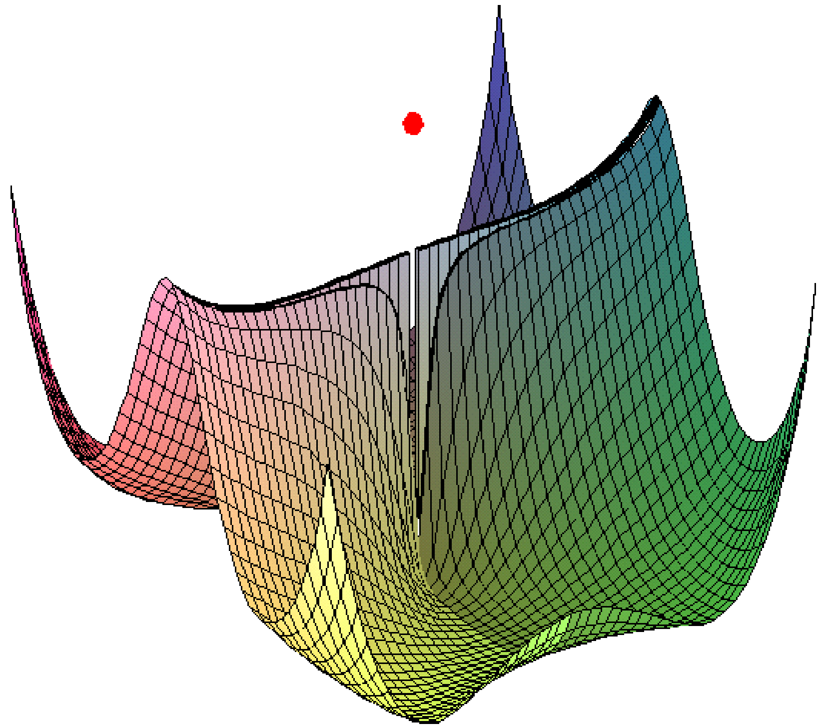




Two-factor, N=11, twin-point IMSPE-optimal design
$(\theta_1, \theta_2) = (0.128, 0.069)$*



Design's dot diagram

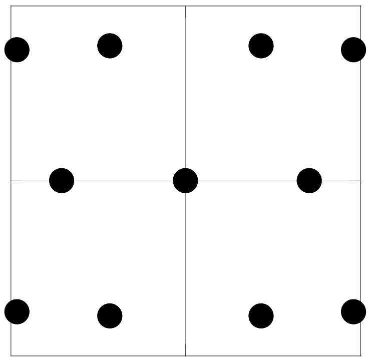


IMSPE vs. δ_1 and δ_2 of one of the twins, with all other points and the center of the twins fixed

* Discovered, c. Y1998 with U. Mich. Systems Programmer Dr. David Woodcock.

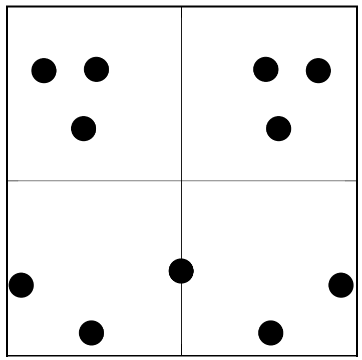
For all designs on this page: θ_1=0.128

membership=1



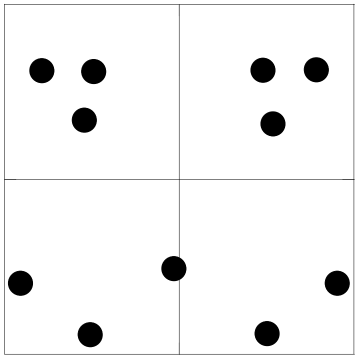
θ_2=0.033

2



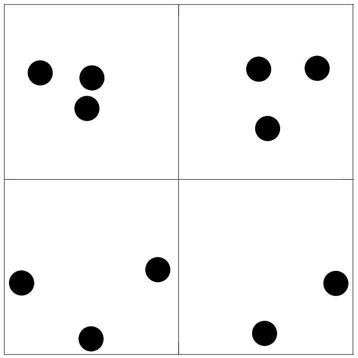
0.035

4



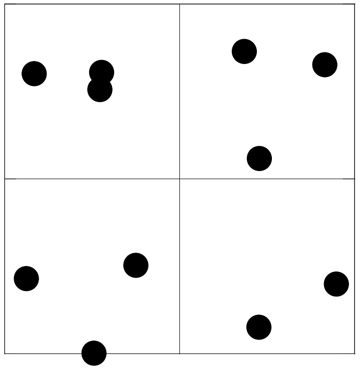
0.037

4



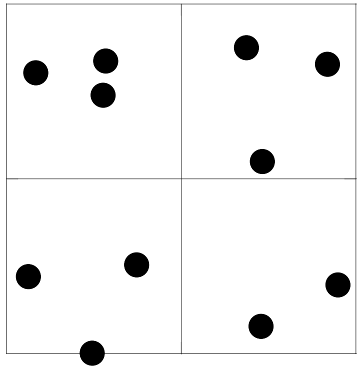
0.038

4 twin



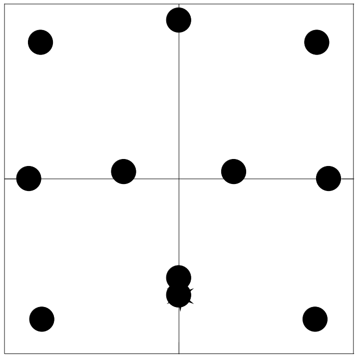
0.050

4



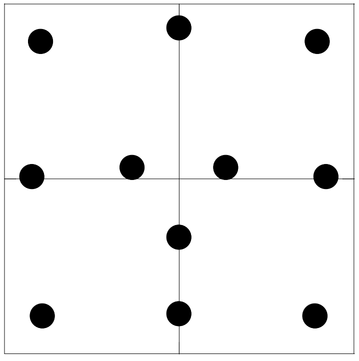
0.056

2 twin

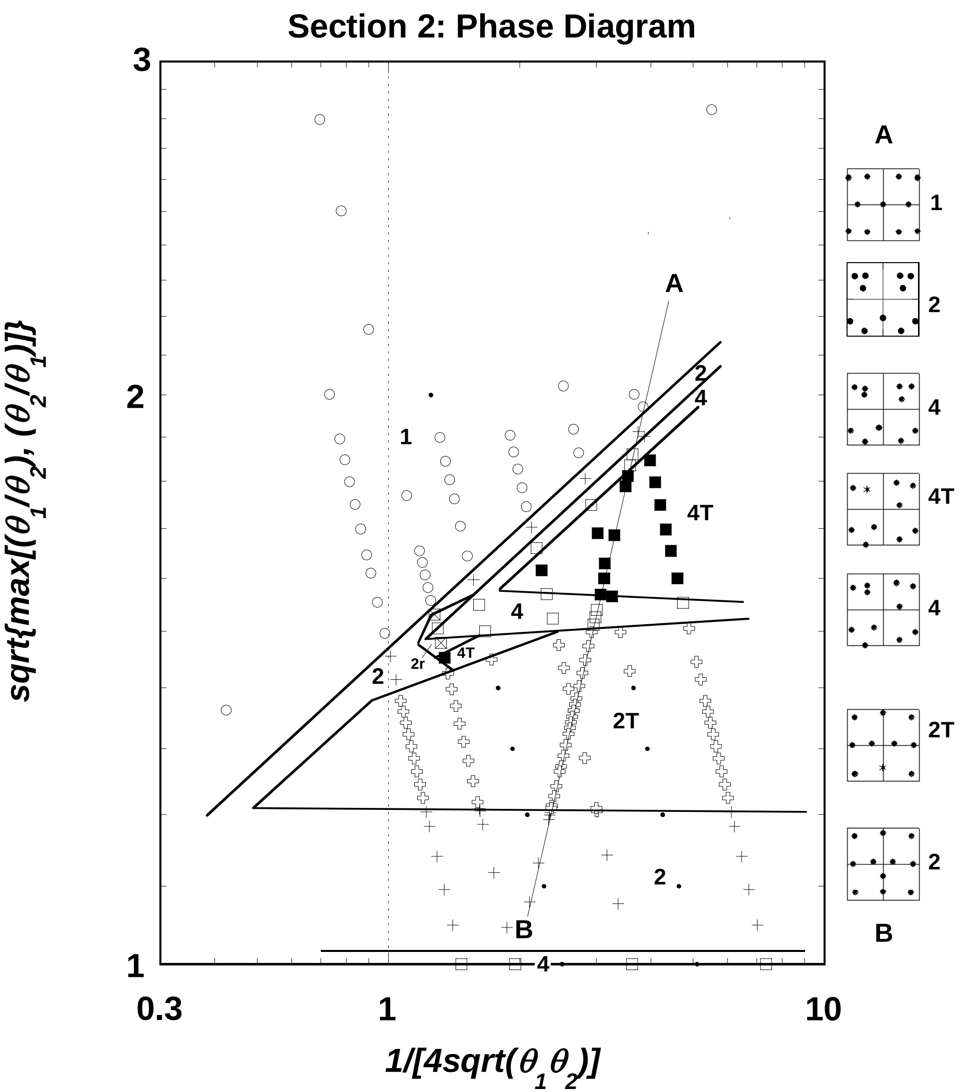


0.069

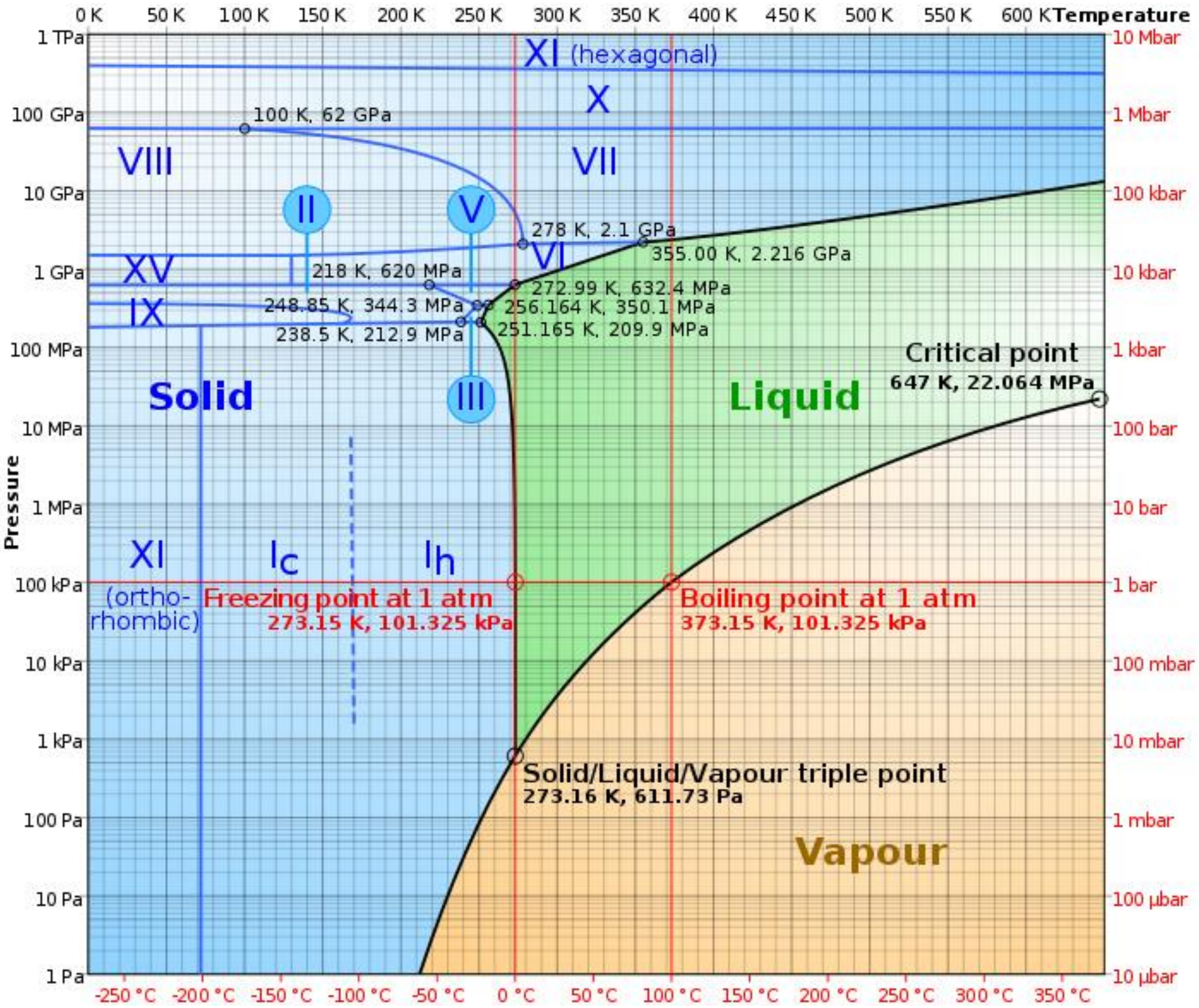
2



0.110

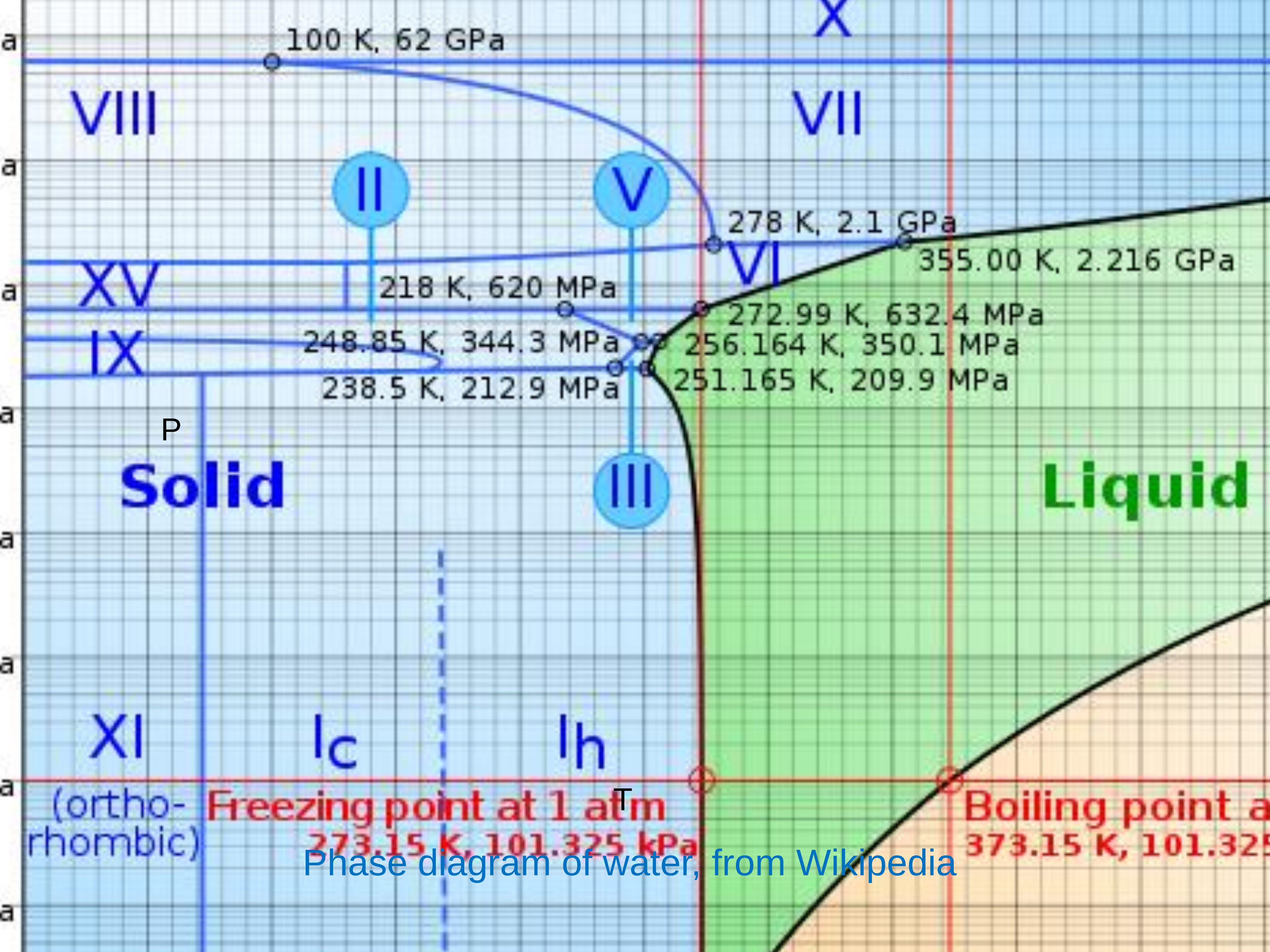

Section 2: Phase Diagram
sqrt{max[(θ1/θ2), (θ2/θ1)]}
1/[4sqrt(θ1θ2)]
3
2
1
0.3
1
10
A
B
1
2
4
4T
2r
2T
A
1
2
4
4T
4
2T
2
B

P



T

Phase diagram of water, from Wikipedia



Phase diagram of water, from Wikipedia

Active theory 1

Example Padé approximant:

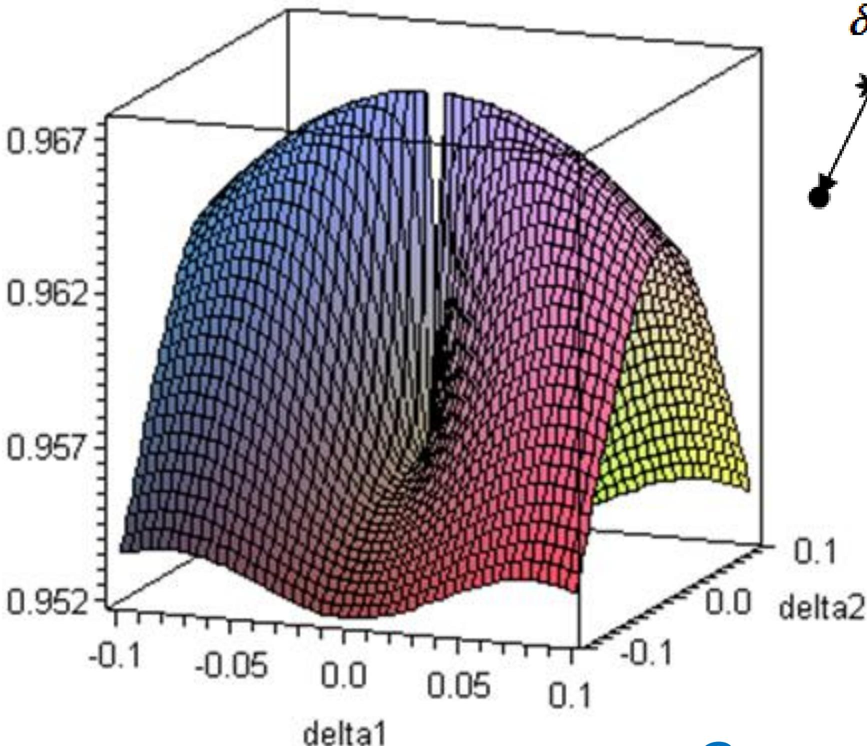
$$P(x_1, x_2) = \frac{\alpha_0 \ +\alpha_1 x_1 + \alpha_2 x_2 \ \cancel{+\alpha_3 {x_1}^2 + \alpha_4 x_1 x_2 + \alpha_5 {x_2}^2 + \cdots}}{\beta_0 \ +\beta_1 x_1 + \beta_2 x_2 \ \cancel{+\beta_3 {x_1}^2 + \beta_4 x_1 x_2 + \beta_5 {x_2}^2 + \cdots}}$$

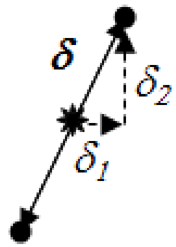
Could be called a "high-degree-truncated rational function."

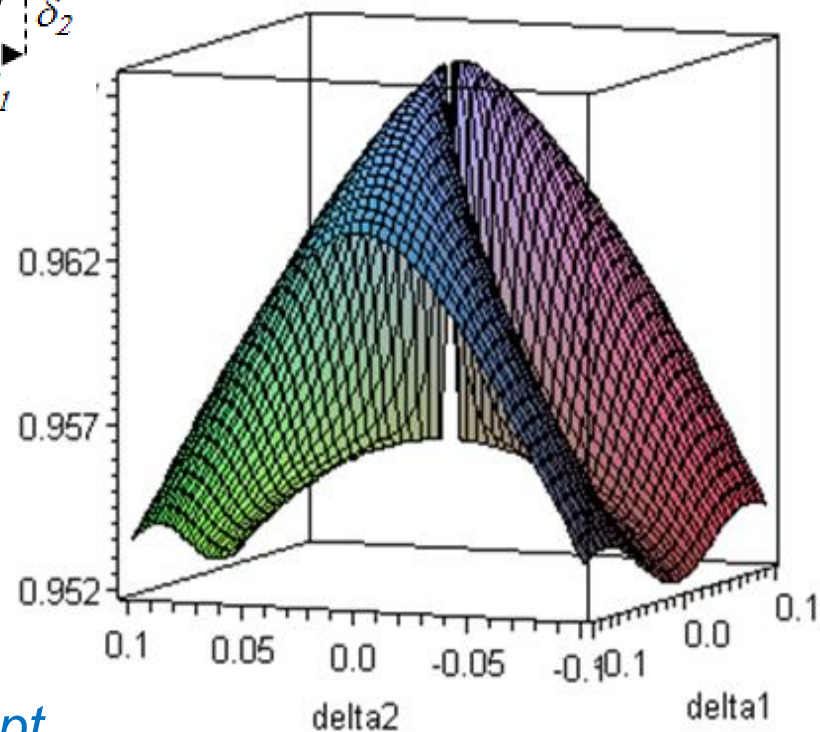
Example twin-point IMSPE functions are, by contrast, "low-degree-truncated rational functions" in the Cartesian coordinates of the half-vectors between twins. We call this new class of "functions" the "Nu class."

$$\mathrm{N}(\delta_1, \delta_2) = \frac{\cancel{\alpha_0 \ +\alpha_1 \delta_1 + \alpha_2 \delta_2} \ +\alpha_3 {\delta_1}^2 + \alpha_4 \delta_1 \delta_2 + \alpha_5 {\delta_2}^2 + \cdots}{\cancel{\beta_0 \ +\beta_1 \delta_1 + \beta_2 \delta_2} \ +\beta_3 {\delta_1}^2 + \beta_4 \delta_1 \delta_2 + \beta_5 {\delta_2}^2 + \cdots}$$

Ex: *IMSE* in the vicinity of a pair of twin points
[-1,1]^2, *N=2,* center of twins at *(0.0,0.6)*

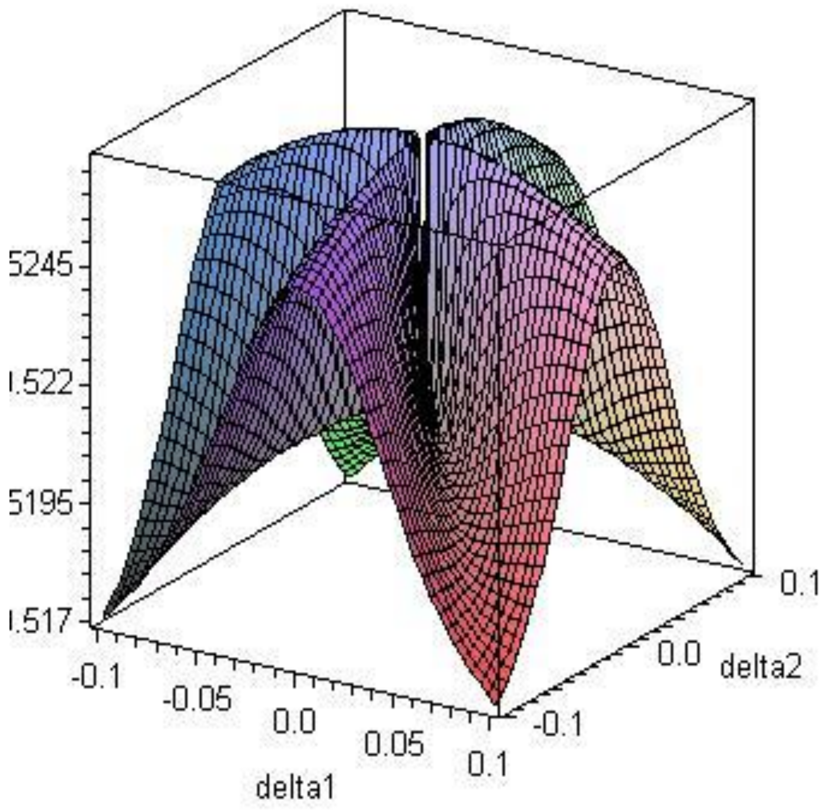






C$^\infty$ *except …*

These figures are from SC and R. Johnson, "Validation of the Twin-Point-Design Concept in the Design of Computer Experiments," Section on Statistical Computing – JSM 2011, pp. 5495-5505.
In the figures, *delta1=2*δ_1 and *delta2=2*δ_2.



Looking to the future: Here is the *IMSE* of three, equispaced, collinear points centered on the origin of $[-1,1]^2$.
As before, $delta1=2\delta_1$ and $delta2=2\delta_2$.

Active theory 2

Sharp phase transitions make these transitions “quantum phase transitions,” despite there being no quantum mechanics, energy, entropy, thermodynamics, dynamics, etc. invoked.

Example: Quantum phase transitions are observed in high-temperature superconductors.

Conjectures

In 1D, there are no free-ranging, IMSPE-optimal, twin-point designs.

The 2D, N=4, free-ranging, IMSPE-optimal system described in this talk has the lowest number of degrees of freedom of any free-ranging, clustered-point design.

Mild-to-wild speculations (Divert your eyes now if you dislike speculations.)

For 2-and-more-D, large-N, free-ranging IMSPE-optimal designs contain myriads of twins, triplets, etc. That is, clustered IMSPE-optimal designs are nearly ubiquitous.

The Nu class has applications to science and engineering. Applications mentioned in our readily found Y2016 arXiv paper are resolution of the “black-hole firewall paradox,” the “notorious node problem” arising in the de Broglie – Bohm formulation of quantum mechanics, and more.

The Nu class leads to a finite-N extension to ordinary thermodynamics, “generalized thermodynamics.” Ordinary thermodynamics is valid only in “the thermodynamic limit,” i.e. for $N \to \infty$.

Parting thought

Session Chair Prof. Weng Kee Wong earlier spoke of “nature-inspired optimization.” We’ve just discussed “optimization-inspired science.”

Invitation

Join us. Collaborate with us. Compete with us. Celebrate both what we don’t understand and what we learn.

Contacts

selden_crary@yahoo.com
saunders@stanford.edu , co-creator of qMinos+X, the Y2015 quadruple-precision optimizer “Minos” now under active development for use in DOE as qMinos+IMSPE.

Other active collaborators

Richard Diehl Martinez, rising junior undergrad., Stanford Univ.
Amin Mobasher, Ph.D., who has a full-time Silicon-Valley day job, but finds time …

Collaboration space

Coupa Café, 538 Ramona Ave, Palo Alto, CA, USA, most days ‘til 23:00