Optimal-design search under the IMSPE objective

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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*

\[ Y = \beta_0 + \beta_1 x + \beta_2 x^2 + \epsilon \]

\[ \epsilon \sim N(0, \sigma_Z^2), \quad N = 5 \]

D-, G-, and I-optimal designs

I\textsubscript{g}–optimal designs for differently weighted integrals

saddle pt.

1 of 2 global min.

*Crary, Hoo, & Tennenhouse
Usual Gaussian-process model
Gaussian covariance matrix: $V_{i,j} = \exp[-\theta_1 (x_{i,1} - x_{j,1})^2 - \theta_2 (x_{i,2} - x_{j,2})^2]$
Response: $Y(x_1, x_2) = \beta_0 + Z$, à la Sacks, Schiller, & Welch 1989; $N = 4$
IMSPE-optimal designs: $\min \int_{\omega_N} E \left[ (\hat{Y} - Y)^2 \right] dx$

Rainbow plot of IMSPE
Phases along $\theta_1 = 0.128$:  

- 4 in-line
- square
- rectangle
- rhombus with twins
- rhombus
Two-factor, N=11, twin-point IMSPE-optimal design
$(\theta_1, \theta_2) = (0.128, 0.069)^*$

Design’s dot diagram

IMSPE vs. $\delta_1$ and $\delta_2$ of one of the twins, with all other points and the center of the twins fixed

For all designs on this page: $\theta_1=0.128$

membership=1

$\theta_2=0.033$

4 twin

4

2 twin

2
Section 2: Phase Diagram

\[ \sqrt{\max\left[\frac{q_1}{q_2}, \frac{q_2}{q_1}\right]} \]

\[ \frac{1}{4\sqrt{q_1q_2}} \]
Phase diagram of water, from Wikipedia
Phase diagram of water, from Wikipedia
Active theory 1

Example Padé approximant:

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

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.”

\[
N(\delta_1, \delta_2) = \frac{\alpha_0 + \alpha_1 \delta_1 + \alpha_2 \delta_2 + \alpha_3 \delta_1^2 + \alpha_4 \delta_1 \delta_2 + \alpha_5 \delta_2^2 + \cdots}{\beta_0 + \beta_1 \delta_1 + \beta_2 \delta_2 + \beta_3 \delta_1^2 + \beta_4 \delta_1 \delta_2 + \beta_5 \delta_2^2 + \cdots}
\]
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 ...
Looking to the future: Here is the IMSE of three, equispaced, collinear points centered on the origin of $[-1,1]^2$. As before, $\delta_1 = 2\delta_1$ and $\delta_2 = 2\delta_2$. 
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