QMC for Sleep Performance

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Talk Outline

- Sleep Performance Model and Computational Tasks

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- Determination of Confidence Region

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  - Safe Height Approximation

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  - Results from Reparameterizations
  - Performance Prediction
- Concluding Remarks

Sleep Performance Model

- Bayesian Model for Sleep Performance (Van Dongen *et al.*, 2007).

$$P(\xi, \lambda, \eta, \nu, \phi, t) = \xi e^{-\rho e^{\nu}(t-t_0)} + \gamma e^{\eta} \sum_{q=1}^{5} a_q \sin(\frac{2q\pi}{24}(t-\phi)) + \kappa + \lambda,$$

$P(\boldsymbol{\theta}, t) = P(\xi, \lambda, \eta, \nu, \phi, t)$ values express cognitive performance in terms of the number of lapses (reaction times exceeding 500 ms) on a 10-min psychomotor vigilance task (PVT),

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  - with variables: t is time (in hours), t_0 time of awakening;
    ξ, initial sleep pressure from prior sleep loss;
    ϕ, temporal alignment of circadian oscillation;
    ν, buildup rate of sleep pressure across time awake;
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  ξ, initial sleep pressure from prior sleep loss;
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  λ, the basal performance capability;
- and fixed parameters from population averages:
  ρ, buildup rate of sleep pressure across time awake;
  γ, amplitude of circadian oscillation; κ, basal performance;
  a_q's, relative amplitudes of harmonics of the circadian oscillation;

Sleep Performance Model Continued

- Likelihood Function: given PVT measurements y_l at times t_l, $l = 1, 2, \ldots, m$, the likelihood for data is

$$L(\xi, \lambda, \eta, \nu, \phi) = \prod_{l=1}^{m} p_N(y_l, P(\xi, \lambda, \eta, \nu, \phi, t_l), \sigma_L^2),$$

with standard mean μ, variance σ^2 univariate normal pdf, $p_N(y, \mu, \sigma^2)$

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  with standard mean μ, variance σ^2 univariate normal pdf, $p_N(y, \mu, \sigma^2)$

- Posterior pdf: uses $\mu = 0$ univariate normal priors for $\nu,\ \eta$, and λ with variances $\sigma_L^2, \sigma_\nu^2, \sigma_\eta^2, \sigma_\lambda^2 = (77.6, 1.15, 0.294, 36.2)$, from population averages; posterior pdf is

$$f(\boldsymbol{\theta}) \equiv f(\xi, \lambda, \eta, \nu, \phi) = (\frac{1}{C})L(\xi, \lambda, \eta, \nu, \phi)p_N(\nu, 0, \sigma_\nu^2)p_N(\eta, 0, \sigma_\eta^2)p_N(\lambda, 0, \sigma_\lambda^2),$$

  where C is a normalization constant.

Computational Tasks

1. Confidence region determination: to find the smallest region in

$$S = \{\boldsymbol{\theta} = (\xi, \lambda, \eta, \nu, \phi) | (\xi, \lambda, \eta, \nu, \phi) \in (-\infty, 0] \times (-\infty, \infty)^3 \times [0, 24]\}$$

containing $100(1-\alpha)\%$ of the (hyper)volume under $f(\boldsymbol{\theta})$.
Given an α with $0 \leq \alpha \leq 1$, define the **confidence region** R_α to be the smallest subset of S satisfying

$$1 - \alpha = \int_{R_\alpha} f(\boldsymbol{\theta}) d\boldsymbol{\theta}.$$

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2. Future performance prediction: given R_α, evaluate the performance function $P(\boldsymbol{\theta}, t)$ over R_α at selected future times t.

Normalization Constant C

$$
\begin{aligned}
C &= \int_{-\infty}^{0}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{24} \\
&\quad L(\xi,\lambda,\eta,\nu,\phi)p_N(nu,0,\sigma_\nu^2)p_N(\eta,0,\sigma_\eta^2)p_N(\lambda,0,\sigma_\lambda^2)d\xi d\nu d\eta d\lambda d\phi, \\
&= \frac{1}{(2\pi)^{\frac{m+3}{2}}}\int_{-\infty}^{0}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{24} e^{-\frac{\nu^2}{2\sigma_\nu^2}-\frac{\eta^2}{2\sigma_\eta^2}-\frac{\lambda^2}{2\sigma_\lambda^2}} \\
&\quad e^{-\frac{\sum_{l=1}^{m}\left(\xi e^{-\rho e^{\nu}(t-t_0)}+\gamma e^{\eta}\sum_{q=1}^{5} a_q\sin(\frac{2q\pi}{24}(t-\phi))+\kappa+\lambda-y_l\right)^2}{2\sigma_L^2}} d\phi d\nu d\eta d\lambda d\xi; \\
C &\equiv \int_{\boldsymbol{\theta}\in S} H(\boldsymbol{\theta})d\boldsymbol{\theta},
\end{aligned}
$$

where

$$H(\boldsymbol{\theta}) \equiv H(\xi,\lambda,\eta,\nu,\phi) = L(\boldsymbol{\theta})p_N(\nu,0,\sigma_\nu^2)p_N(\eta,0,\sigma_\eta^2)p_N(\lambda,0,\sigma_\lambda^2).$$

is the unnormalized posterior density.

Safe Height h_α

- Background:
  the boundary of smallest confidence region for a continuous pdf always projects to a level (fixed-height) contour on the surface of the pdf (Box and Tiao, 1992).
- Definition:
  let h_α denote the **safe height** of this contour, so that the **confidence region** R_α is implicitly defined by

$$R_\alpha = \{\boldsymbol{\theta} \mid \boldsymbol{\theta} \in S,\ H(\boldsymbol{\theta}) \geq h_\alpha\}.$$

Simple Monte Carlo Methods

- Use truncated domain $\hat{S} = [c_1, d_1] \times [c_2, d_2] \times [c_3, d_3] \times [c_5, d_4] \times [c_5, d_5]$, with all limits finite, and $d_1 = 0$, $[c_5, d_5] = [0, 24]$. Other limits determined by investigating decay of $H(\boldsymbol{\theta})$ for large values of $-\xi$, $\pm\nu$, $\pm\eta$ and $\pm\lambda$ (Smith et al., 2009). Then, with $W = \prod_{k=1}^{5}(d_k - c_k)$,

$$C \approx \int_{\boldsymbol{\theta} \in \hat{S}} H(\boldsymbol{\theta}) d\boldsymbol{\theta} = W \int_0^1 \int_0^1 \int_0^1 \int_0^1 \int_0^1 H(\mathbf{c} + (\mathbf{d} - \mathbf{c})\mathbf{x}) d\mathbf{x}.$$

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- Monte Carlo (MC) estimate for C is

$$\hat{C}_N = \frac{W}{N}\sum_{i1}^{N} H(\mathbf{c}+(\mathbf{d}-\mathbf{c})\mathbf{x}_i),$$

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$$\hat{C}_N = \frac{W}{N}\sum_{i1}^{N} H(\mathbf{c}+(\mathbf{d}-\mathbf{c})\mathbf{x}_i),\ E_N = \left(\frac{1}{N(N-1)}\sum_{i=1}^{N}(WH(\mathbf{c}+(\mathbf{d}-\mathbf{c})\mathbf{x}_i) - \hat{C}_N)^2\right)$$

given $\mathbf{x}_i$'s with uniform random components ($x_{ki} \sim U(0,1)$), and with E_N typically scaled by 3 to give approximate 99% confidence.

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$$C \approx \int_{\theta \in \hat{S}} H(\theta) d\theta = W \int_0^1 \int_0^1 \int_0^1 \int_0^1 \int_0^1 H(\mathbf{c} + (\mathbf{d} - \mathbf{c})\mathbf{x}) d\mathbf{x}.$$

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  given $\mathbf{x}_i$'s with uniform random components ($x_{ki} \sim U(0, 1)$), and with E_N typically scaled by 3 to give approximate 99% confidence.
- MC methods using N points have errors that are typically $O(1/N^{\frac{1}{2}})$, a convergence rate which is too slow for many problems.

Quasi-Monte Carlo (QMC) Methods

- Use QMC points instead of MC points for $\hat{C}_N$, for example $\mathbf{x}_i = \{i\,\mathbf{Z}\}$, where $\mathbf{Z}$ is an appropriately chosen *generating* vector, and $\{\cdot\}$ denotes componentwise fractional parts.
- Tests will use *Kronecker* ("Richtmyer" prime square roots sequence, see Drmota and Tichey, 1997, Fang and Wang, 1994) and *lattice* (see Sloan and Joe, 1994, Nuyens and Cools, 2006) sequences.

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- Error estimates from randomly shifted sets (or batches) of QMC points; Given $\mathbf{u}$ with components $u_i \sim U(0,1)$, use QMC approximations

$$\hat{C}_N(\mathbf{u}) = \frac{W}{N}\sum_{i1}^{N} H(\mathbf{c} + (\mathbf{d} - \mathbf{c})(\{\mathbf{x}_i + \mathbf{u}\})).$$

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Then an unbiased **MCQMC** approximation for C is (with standard error)

$$\hat{C}_{N,K} = \frac{1}{K}\sum_{k=1}^{K}\hat{C}_N(\mathbf{u}_k),\ \ E_{N,K} = \Big(\frac{1}{K(K-1)}\sum_{k=1}^{K}(\hat{C}_N(\mathbf{u}_k) - \hat{C}_{N,K})^2\Big)^{\frac{1}{2}}.$$

Note: K is usually chosen to be small (e.g. $K = 10$) relative to N;
N is increased to efficiently reduce error in $\hat{C}_{K,N}$.

Safe Height Approximation

- If C is approximated using equal-weight numerical integration method

$$C \approx \hat{C} = \frac{W}{N} \sum_{i=1}^{N} H(\boldsymbol{\theta}_i),$$

approximate h_α value is determined from the smallest $H(\boldsymbol{\theta}_i)$ value in the set containing the largest $100(1-\alpha)\%$ of $H(\boldsymbol{\theta}_i)$ values.
Determine $H(\boldsymbol{\theta}_{(i)})$ sequence from sorted (ascending order) $H(\boldsymbol{\theta}_i)$'s and

$$H_\alpha = H(\boldsymbol{\theta}_{(i^*)}), \text{ with } i^* = \lceil \alpha N \rceil,$$

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defines an approximation to safe height h_α.

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defines an approximation to safe height h_α.

- Let $\hat{h}_{\alpha,N}(\mathbf{u})$ denote approximate h_α using a $\mathbf{u}$ randomly shifted QMC (or MC) point set; then unbiased MCQMC estimates for h_α are averages

$$\hat{h}_{\alpha,N,K} = \frac{1}{K} \sum_{k=1}^{K} \hat{h}_{\alpha,N}(\mathbf{u}_k);$$

standard errors provide error estimates.

Future Performance Prediction

- Given $H(\boldsymbol{\theta}_{(i)}(\mathbf{u}))$'s, from a **u** randomly shifted QMC (or MC) point set, define the **confidence set** $\hat{R}_{\alpha,N}(\mathbf{u})$

$$\hat{R}_{\alpha,N}(\mathbf{u}) = \{\boldsymbol{\theta}_{(i)}(\mathbf{u})) \mid i \geq \lceil \alpha N \rceil\}.$$

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$$\hat{R}_{\alpha,N}(\mathbf{u}) = \{\boldsymbol{\theta}_{(i)}(\mathbf{u})) \mid i \geq \lceil \alpha N \rceil\}.$$

- Approximate future performance prediction: given $\hat{R}_{\alpha,N}(\mathbf{u})$'s evaluate the performance function $P(\boldsymbol{\theta}, t)$ over $\hat{R}_{\alpha,N}(\mathbf{u})$'s at selected future times t.

Tests with No Transformations

- Data for all tests taken from Van Dongen et al. (2007, individual C) with 24 past performance measurements $\{(t_l, y_l) | l = 1, \ldots, 24\}$, for 48 hours of total sleep deprivation, $t_l = 5.5 + 2l$, and

$$\mathbf{y} = (8\ 17\ 19\ 19\ 13\ 15\ 11\ 22\ 9\ 33\ 24\ 27\ 34\ 36\ 25\ 31\ 39\ 31\ 38\ 46\ 39\ 34\ 27\ 46).$$

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- The maximum (mode) for the posterior $H(\boldsymbol{\theta})$ occurs approximately at $\boldsymbol{\theta} \equiv \boldsymbol{\mu} = (-32.725,\ 8.2011,\ -.15275,\ .48695,\ 4.4711)$.
- Truncated domain is

$$\hat{S} = [-60, 0] \times [-20, 40] \times [-4, 4] \times [-3, 3] \times [0, 24]$$

(see Smith et al., 2009), based on investigation of the rates of decrease in $H(\boldsymbol{\theta})$ for large values of $-\xi$, $\pm\nu$, $\pm\eta$ and $\pm\lambda$.

Tests with No Transformations Continued

- Some results use MC, and two MCQMC methods:
  MCQMCK uses Richtmyer (square roots of primes) generators;
  MCQMCL uses lattice rule generators, from Nuyens-Cools (2006) CBC.

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Table: Computation of $\hat{C}$ using MC and MCQMC Methods

NK	MC	Error	MCQMCK	Error	MCQMCL	Error
100000	.304	.122	.3176	.0367	.3088	.01680
200000	.315	.075	.3105	.0367	.2996	.03602
400000	.286	.042	.2938	.0302	.2916	.02611
800000	.296	.023	.2941	.0174	.3008	.00166
$\hat{h}_{\alpha,80000,10}$	1.67e-6	2.9e-7	1.6e-6	1.1e-7	1.74e-6	6e-8

Tests done with $K = 10$, and $3 \times E_{N,K}$ used for the **Error** columns.
Note: $\hat{C}$ approximations in Tables scaled by $(2\pi)^{\frac{m+3}{2}}$.

- Results show the superiority of QMC methods, particularly lattice rules.

Tests with Standardizing Transformation

- Consider standardizing transformation $\theta(\mathbf{x}) = \boldsymbol{\mu} + L\mathbf{y}$ where L is Cholesky factor for posterior covariance matrix $\boldsymbol{\Sigma}$ ($\boldsymbol{\Sigma} = LL^t$), given by $\boldsymbol{\Sigma} = G^{-1}$, when G is Hessian for $-\log(H(\boldsymbol{\theta}))$ at $\boldsymbol{\theta} = \boldsymbol{\mu}$.
- Complication: $H(\boldsymbol{\theta})$ is (slowly varying) periodic (not decaying) in ϕ, so full 5-variable model is not directly applicable.
- However, with varying $\phi \in [0, 24]$, $(\xi, \nu, \eta, \lambda)$ components of mode and, 4×4 $\boldsymbol{\Sigma}$'s do not change significantly.
- So use $\theta(\mathbf{y}) = \boldsymbol{\mu} + L\mathbf{y}$, where L is Cholesky factor for $\boldsymbol{\Sigma}$ determined from approximate Hessian of $-\log(H(\boldsymbol{\theta}))$ with fixed $\phi = 4.4711$; then

$$L \approx \begin{bmatrix} 6.3834 & 0 & 0 & 0 & 0 \\ -2.1172 & 3.1661 & 0 & 0 & 0 \\ -.092616 & -.03576 & .40832 & 0 & 0 \\ -.000407 & -.27182 & .01002 & .17602 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Tests with Standardizing Transformation Continued

- With standardizing transformation $\theta(\mathbf{x}) = \boldsymbol{\mu} + L\mathbf{y}$

$$C \approx |L| \int_{-d}^{-\mu_1/l_{11}} \int_{-d}^{d} \int_{-d}^{d} \int_{-d}^{d} \int_{0}^{24} H(\boldsymbol{\mu} + L\mathbf{y}) d\mathbf{y}$$

where $|L| = det(L) = \prod_{k=1}^{5} l_{kk}$, $d = 5$ is a selected cutoff value, and upper y_1 limit μ_1/l_{11} corresponds to $\xi = \mu_1 + l_{11}y_1 = 0$.

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Table: Standardized $\hat{C}$ Computation with MC and MCQMC Methods

NK	MC	Error	MCQMCK	Error	MCQMCL	Error
100000	.288	.029	.2986	.0490	.30135	.00666
200000	.304	.027	.3007	.0030	.29955	.00211
400000	.295	.023	.3022	.0022	.30275	.00351
800000	.298	.011	.3003	.0009	.30035	.00009
$\hat{h}_{\alpha,80000,10}$	1.69e-6	9e-8	1.74e-6	4e-8	1.73e-6	3e-8

- Standardized results are generally much more accurate than unstandardized results and also show superiority of QMC methods.

Tests with Standardizing & SR Transformation

- First transform ξ to $w \in (-\infty, \infty)$ with $\xi = -e^w$, then use standardizing transformation for $H(-e^w, \lambda, \eta, nu, \phi)e^w$ (extra e^w because $d\xi = -e^w dw$. Then $\boldsymbol{\mu} \approx (3.5261,\ 8.6272,\ -.13415,\ .48632,\ 4.5866)$, and

$$L \approx \begin{bmatrix} .18491 & 0 & 0 & 0 & 0 \\ 2.0887 & 3.2427 & 0 & 0 & 0 \\ .094273 & -.037663 & .40780 & 0 & 0 \\ .000021 & -.27323 & .00993 & .17107 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

and

$$C = |L| \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{0}^{24} H(\theta(\mathbf{w}(\mathbf{y})))e^{w_1(y_1)} d\mathbf{y}$$

with $\theta(\mathbf{w})) = (-e^{w_1}, w_2, w_3, w_4, w_5)$, and $\mathbf{w}(\mathbf{y}) = \boldsymbol{\mu} + L\mathbf{y}$.

Tests with Standardizing & SR Transformation Cont.

- Next use "spherical-radial" (SR) transformation for first 4 **y** components $(y_1, y_2, y_3, y_4) = r(z_1, z_2, z_3, z_4)$ with $r \in [0, \infty)$ and $\mathbf{z} \in U_4$, the surface of the unit 4-sphere, $U_4 = \{\ \mathbf{z} \mid z_1^2 + z_2^2 + z_3^2 + z_4^2 = 1\ \}$. Then

$$C \approx |L| \int_0^d \int_{||\mathbf{z}||_2=1} \int_0^{24} H(\theta(\mathbf{w}(\mathbf{y}(\mathbf{z}))))e^{w_1(y_1(\mathbf{z}))} r^3 dr d\mathbf{z} dy_5,$$

where $d\mathbf{z}$ is U_4 measure; cutoff value d replaces ∞ upper r limit.

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  where $d\mathbf{z}$ is U_4 measure; cutoff value d replaces ∞ upper r limit.

- MCQMC methods need $\mathbf{x} \in [0, 1]^5$ variables, so use (see Fang and Wang, 1994)

$$(z_1, \dots, z_4) = \Big(\sqrt{x_1}(\sin(2\pi x_2), \cos(2\pi x_2)), \sqrt{1 - x_1}(\sin(2\pi x_3), \cos(2\pi x_3))\Big),$$

  with constant Jacobian $2\pi^2$, $r = d\ x_4$ and $y_5 = 24x_5$, so that

$$\hat{C}_N = \frac{24d^4|L|2\pi^2}{N} \sum_{i=1}^{N} H(\theta(\mathbf{w}(\mathbf{y}(\mathbf{z}(\mathbf{x}_i)))))e^{w_1(y_1(\mathbf{z}(\mathbf{x}_i)))} x_4^3,$$

  can be used for MC or QMC approximations to C.

Tests with Standardizing & SR Transformation Cont.

- Results for MC, MCQMCK and MCQMCL methods, with standardizing & SR tranformation, for cutoff $d = 6$.

Table: Standardized SR $\hat{C}$ Computation with MC and MCQMC Methods

NK	MC	Error	MCQMCK	Error	MCQMCL	Error
100000	.3033	.0079	.3002	.0006	.30013	.00027
200000	.2989	.0050	.2999	.0003	.29995	.00019
400000	.2999	.0026	.3000	.0004	.30003	.00006
800000	.2997	.0026	.3000	.0001	.30002	.00004
$\hat{h}_{\alpha,80000,10}$	.1988	.0024	.1992	.0015	.2002	.0008

- Results are even more accurate than previous standardized results; the h_α approximations differ because of transformations, but R_α confidence sets, can still be used for performance prediction.

Tests with Standardizing & SR Transformation Cont.

- Accuracy levels in Table from standardized, SR transformed lattice-rule QMC combination are not typically needed for practical performance prediction. Further tests have shown that sufficient accuracy is obtained with values for $NK \approx 10000$.

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- Accuracy levels in Table from standardized, SR transformed lattice-rule QMC combination are not typically needed for practical performance prediction. Further tests have shown that sufficient accuracy is obtained with values for $NK \approx 10000$.
- Also studied other transformations of $(\xi, \lambda, \eta, \nu)$ variables based on multivariate normal model $H(\theta(\mathbf{y})) \sim e^{-\mathbf{y}^t\mathbf{y}/2}$ (and other related statistical distribution models) with, for example, $x_i = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{y_i} e^{-t_i^2/2} dt$. Results using these models as a basis for transforming $(\xi, \nu, \eta, \lambda)$ variables resulted in less accurate $\hat{C}$ approximations, given the same amount of computational work (NK values).

Performance Prediction Results

- Predicted performance computed using data collected during C computation of C, where K $\hat{R}_{\alpha,N}$ sets are also computed.
- Given a set $\hat{R}_{\alpha,N}$ containing M $\boldsymbol{\theta}_i$ points, and a future time t, compute predicted **average** $\hat{P}_N(t)$, **minimum** $\underline{P}_N(t)$, and **maximum** $\overline{P}_N(t)$ performance, using

$$\hat{P}_N(t) = \frac{1}{M} \sum_{\boldsymbol{\theta}_i \in \hat{R}_{\alpha,N}} P(\boldsymbol{\theta}_i, t), \;\; \underline{P}_N(t) = \min_{\boldsymbol{\theta}_i \in \hat{R}_{\alpha,N}} P(\boldsymbol{\theta}_i, t), \;\; \overline{P}_N(t) = \max_{\boldsymbol{\theta}_i \in \hat{R}_{\alpha,N}} P(\boldsymbol{\theta}_i, t).$$

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- Figure shows PVT lapse data values for individual C from Dongen et al. (2007) followed by average (over K $\hat{R}_{\alpha,N}$ sets) predicted $\hat{P}_N(t)$ values every hour for 24 additional hours; for each $\hat{P}_N(t)$ value, error bars computed using $\underline{P}_N(t)$ and $\overline{P}_N(t)$ values provide confidence intervals. Data for ($\hat{P}_N(t)$, confidence interval) values in Figure were collected during standardized SR computations with $NK = 100000$.

Performance Prediction Results

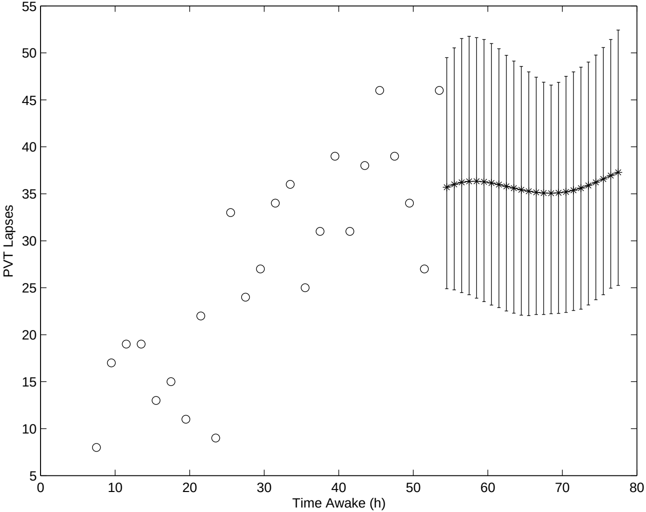

Figure: Predicted Cognitive Performance (PVT Lapse) with Confidence Intervals: 'o' points denote individual data values; '*' points denote predicted values

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- New method makes it possible to provide confidence intervals for Bayesian model predictions in real time.

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