

S1 Appendix.

Dual Unscented Kalman Filter

A dual unscented Kalman filter (UKF) was used for simultaneous estimation and tracking of model states and parameters. This methodology approximates the distribution of states by running the model with a simplex of sigma points as initial conditions. The process begins by initializing state and parameter estimates and covariances for a model system with n_x states and n_w estimated parameters.

$$\hat{x}_0 = \mathbb{E}[x_0] \quad (1)$$

$$\hat{w}_0 = \mathbb{E}[w_0] \quad (2)$$

$$P_{x_0} = \mathbb{E}[(x_0 - \hat{x}_0)(x_0 - \hat{x}_0)^T] \quad (3)$$

$$P_{w_0} = \mathbb{E}[(w_0 - \hat{w}_0)(w_0 - \hat{w}_0)^T] \quad (4)$$

Weighting schemes W for determining mean state estimates and covariances were assigned using the methodology described by Wan and van der Merwe [1].

Set weights for the state filter:

$$\lambda_x = \alpha_x^2(n_x + \kappa_x) - n_x \quad (5)$$

$$W_{x,0}^{(m)} = \frac{\lambda_x}{n_x + \lambda_x} \quad (6)$$

$$W_{x,0}^{(c)} = \frac{\lambda_x}{n_x + \lambda_x} + (1 - \alpha_x^2 + \beta_x) \quad (7)$$

$$W_{x,i}^{(m)} = W_{x,i}^{(c)} = \frac{\lambda_x}{2(n_x + \lambda_x)}, \quad i = 1, \dots, 2n_x \quad (8)$$

Set augmented weights for the state filter:

$$W_{x,0}^{\text{aug},(m)} = \frac{\lambda_x}{2n_x + \lambda_x} \quad (9)$$

$$W_{x,0}^{\text{aug},(c)} = \frac{\lambda_x}{2n_x + \lambda_x} + (1 - \alpha_x^2 + \beta_x) \quad (10)$$

$$W_{x,i}^{\text{aug},(m)} = W_{x,i}^{\text{aug},(c)} = \frac{\lambda_x}{2(2n_x + \lambda_x)}, \quad i = 1, \dots, 4n_x \quad (11)$$

Set weights for the parameter filter:

$$\lambda_w = \alpha_w^2(n_w + \kappa_w) - n_w \quad (12)$$

$$W_{w,0}^{(m)} = \frac{\lambda_w}{n_w + \lambda_w} \quad (13)$$

$$W_{w,0}^{(c)} = \frac{\lambda_w}{n_w + \lambda_w} + (1 - \alpha_w^2 + \beta_w) \quad (14)$$

$$W_{w,i}^{(m)} = W_{w,i}^{(c)} = \frac{\lambda_w}{2(n_w + \lambda_w)}, \quad i = 1, \dots, 2n_w \quad (15)$$

UKF State Filter

The state filter of the dual UKF uses the most recent estimates of parameter means w_{k-1} , as well as the most recent estimate of state mean, \hat{x}_{k-1} , and state covariance $P_{x_{k-1}}$ to approximate the posterior distribution of the model's mapping of the current state distribution into the future. First, compute sigma points around the current state

estimate:

$$\chi_{0,k-1} = \hat{x}_{k-1} \quad (16)$$

$$\chi_{i,k-1} = \hat{x}_{k-1} + (\sqrt{(n_x + \lambda_x)P_{x_{k-1}}})_i, \quad i = 1, \dots, n_x \quad (17)$$

$$\chi_{i,k-1} = \hat{x}_{k-1} - (\sqrt{(n_x + \lambda_x)P_{x_{k-1}}})_i, \quad i = n_x + 1, \dots, 2n_x, \quad (18)$$

where $(\sqrt{(n_x + \lambda_x)P_{x_{k-1}}})_i$ is the i^{th} column of the matrix square root. Apply constraints for real positivity to sigma points.

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for  $j = 1, \dots, n_x$  do
  if  $\chi_{i,k-1}^j < 0$  then
     $\chi_{i,k-1}^j = \min_i \Re(\chi_{i,k-1}^j)$ 
     $\chi_{i,k-1}^j = \max(0, \chi_{i,k-1}^j)$ 
  end if
end for

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Compute the posterior sigma points $\chi_{i,k|k-1}^*$ using the mapping (the model) f .

$$\hat{w}_k = \hat{w}_{k-1} \quad (19)$$

$$\chi_{i,k|k-1}^* = f(\chi_{i,k-1}, \hat{w}_{k-1}) \quad (20)$$

Compute the mean and covariance of posterior sigma points $\chi_{i,k|k-1}^*$, and add the assumed model process noise R_v to the posterior covariance estimate:

$$\hat{x}_{k|k-1}^* = \sum_{i=0}^{2n_x} W_{x,i}^{(m)} \chi_{i,k|k-1}^* \quad (21)$$

$$P_{x_{k|k-1}} = \sum_{i=0}^{2n_x} W_{x,i}^{(c)} (\chi_{i,k|k-1}^* - \hat{x}_{k|k-1}^*)(\chi_{i,k|k-1}^* - \hat{x}_{k|k-1}^*)^T + R_v \quad (22)$$

Augment posterior sigma points:

$$\chi_{i,k|k-1} = \chi_{i,k|k-1}^*, \quad i = 0, \dots, 2n_x \quad (23)$$

$$\chi_{i,k|k-1} = \chi_{0,k|k-1}^* + (\sqrt{(n_x + \lambda_x)P_{x_{k|k-1}}})_i, \quad i = 2n_x + 1, \dots, 3n_x \quad (24)$$

$$\chi_{i,k|k-1} = \chi_{0,k|k-1}^* - (\sqrt{(n_x + \lambda_x)P_{x_{k|k-1}}})_i, \quad i = 3n_x + 1, \dots, 4n_x \quad (25)$$

Compute measurement forecast:

$$\hat{x}_{k|k-1} = \sum_{i=0}^{4n_x} W_{x,i}^{\text{aug},(m)} \chi_{i,k|k-1} \quad (26)$$

$$\mathcal{Y}_{k|k-1} = h(\chi_{k|k-1}, \hat{w}_k) \quad (27)$$

$$\hat{y}_{k|k-1} = \sum_{i=0}^{4n_x} W_{x,i}^{\text{aug},(m)} \mathcal{Y}_{i,k|k-1} \quad (28)$$

Compute Kalman gain, where R_n denotes assumed measurement noise.

$$P_{y_k} = \sum_{i=0}^{4n_x} W_{x,i}^{\text{aug},(c)} (\mathcal{Y}_{i,k|k-1} - \hat{y}_{k|k-1}) (\mathcal{Y}_{i,k|k-1} - \hat{y}_{k|k-1})^T + R_n \quad (29)$$

$$P_{x_k y_x} = \sum_{i=0}^{4n_x} W_{x,i}^{\text{aug},(c)} (\chi_{i,k|k-1} - \hat{x}_{k|k-1}^*) (\mathcal{Y}_{i,k|k-1} - \hat{y}_{k|k-1})^T \quad (30)$$

$$K_k = P_{x_k y_x} P_{y_k}^{-1} \quad (31)$$

Update state covariance:

$$P_{x_k} = P_{x_{k|k-1}} - K_k P_{y_k} K_k^{-1} \quad (32)$$

Update state estimate:

$$\hat{x}_k = \hat{x}_{k|k-1} + K_k (y_k - \hat{y}_{k|k-1}), \quad (33)$$

where y_k is the k^{th} measurement.

UKF Parameter Filter

The parameter filter of the dual UKF uses the most recent estimates of parameter means, w_{k-1} , and their covariance $P_{w_{k-1}}$, as well as state estimate, \hat{x}_{k-1} , to approximate the posterior distribution of parameters, w_k [2]. This is done by creating sigma points that approximate the distribution of w_k , and collecting the measurement forecasts created by the state mappings performed with each of the parameter sigma points, $\mathcal{W}_{i,k|k-1}$.

First, iterate parameter estimates and their covariance:

$$\hat{w}_{k|k-1} = \hat{w}_{k-1} \quad (34)$$

$$P_{w_{k|k-1}} = P_{w_{k-1}} + Q_{w_{k-1}}, \quad (35)$$

where

$$Q_{w_{k-1}} = \text{diag}((\tilde{\lambda}^{-1} - 1)P_{w_{k-1}}), \quad (36)$$

and $\text{diag}(\cdot)$ indicates setting off-diagonal entries to 0.

Compute sigma points around parameter estimate:

$$\mathcal{W}_{0,k|k-1} = \hat{w}_{k|k-1} \quad (37)$$

$$\mathcal{W}_{i,k|k-1} = \hat{w}_{k|k-1} + (\sqrt{(n_w + \lambda_w)P_{w_{k|k-1}}})_i, \quad i = 1, \dots, n_w \quad (38)$$

$$\mathcal{W}_{i,k|k-1} = \hat{w}_{k|k-1} - (\sqrt{(n_w + \lambda_w)P_{w_{k|k-1}}})_i, \quad i = n_w + 1, \dots, 2n_w \quad (39)$$

Apply constraints for real positivity to sigma points.

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for  $j = 1, \dots, n_w$  do
  if  $\mathcal{W}_{i,k-1}^j < 0$  then
     $\mathcal{W}_{i,k-1}^j = \min_i \Re(\mathcal{W}_{i,k-1}^j)$ 
     $\mathcal{W}_{i,k-1}^j = \max(0, \mathcal{W}_{i,k-1}^j)$ 
  end if
end for

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Compute measurement forecast:

$$\mathcal{Y}_{i,k|k-1} = h(f(\hat{x}_{k-1}, \mathcal{W}_{i,k|k-1}), \mathcal{W}_{i,k|k-1}) \quad (40)$$

Compute Kalman gain:

$$P_{y_k} = \sum_{i=0}^{2n_w} W_{w,i}^{(c)} (\mathcal{Y}_{i,k|k-1} - \hat{y}_{k|k-1}) (\mathcal{Y}_{i,k|k-1} - \hat{y}_{k|k-1})^T + R_n \quad (42)$$

$$P_{w_k y_x} = \sum_{i=0}^{2n_w} W_{w,i}^{(c)} (\mathcal{W}_{i,k|k-1} - \hat{w}_{k|k-1}) (\mathcal{Y}_{i,k|k-1} - \hat{y}_{k|k-1})^T \quad (43)$$

$$K_k = P_{w_k y_x} P_{y_k}^{-1} \quad (44)$$

Update parameter covariance:

$$P_{w_k} = P_{w_{k|k-1}} - K_k P_{y_k} K_k^{-1} \quad (45)$$

Update parameter estimate:

$$\hat{w}_k = \hat{w}_{k|k-1} + K_k (y_k - \hat{y}_{k|k-1}), \quad (46)$$

where y_k is the k^{th} measurement.

Table 1. Full list of parameters used in the dual UKF, where the ultradian model has 6 states and the meal model has 12 states. Values for α were determined via ad hoc experimentation, and were important for stable covariance estimates.

Dual UKF parameters		
Parameter	Value	Meaning
n_x	12 or 6	Number of model states
n_w	3	Number of estimated model parameters
α_x	0.4	State sigma point weighting constant
α_w	0.3	Parameter sigma point weighting constant
β_x	2	Parameter sigma point weighting constant
β_w	2	State sigma point weighting constant
κ_x	$3 - n_x$	Parameter sigma point weighting constant
κ_w	0	State sigma point weighting constant
$\tilde{\lambda}$	0.9975	"Forget" factor for parameter covariance
q_v	0.4	State sigma point weighting constant
q_n	0.01	State sigma point weighting constant
R_v	$\text{diag}((q_v \cdot v_{\text{all}})^2)$	Assumed process noise covariance
R_n	$\text{diag}((q_n \cdot v_{\text{obs}})^2)$	Assumed measurement noise covariance

The assumed process and measurement noise variance, R_v and R_n , respectively, were computed as fractions (q_v and q_n) of the time-averaged state values, v_{all} . We considered model process noise to have a standard deviation of 40% of v_{all} . R_n was considered to have a standard deviation of 1% of average measurement values; although typical glucometers have error closer to 10%, we found it advantageous to artificially lower R_n in order to weight measurements more severely and, thus, train the model more quickly. Time-averaged state values, v_{all} , were computed using simulated initial states and nutrition.

Meal Model average state values

$$v_{\text{all}} = \begin{bmatrix} 219.85 \\ 164.08 \\ 8.88 \\ 2.46 \\ 39.26 \\ 37.00 \\ 6307.52 \\ 7914.55 \\ 3103.47 \\ 19.08 \\ 5.413 \\ 0.85 \end{bmatrix} v_{\text{obs}} = 219.85 \tag{47}$$

Ultradian Model average state values

$$v_{\text{all}} = \begin{bmatrix} 82.24 \\ 191.57 \\ 11235.00 \\ 82.02 \\ 82.27 \\ 81.86 \end{bmatrix} v_{\text{obs}} = 11235.00 \tag{48}$$

References

1. Wan EA, Merwe RVD. The Unscented Kalman Filter. In: Kalman Filtering and Neural Networks. Wiley; 2001. p. 221–280.
2. Gove J, Hollinger D. Application of a dual unscented Kalman for simultaneous state and parameter estimation problems of surface-atmospher exchange. J Geophys Res. 2006;111:DO8S07.