Learning and Control using Gaussian Processes

Towards bridging machine learning and controls for physical systems

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Gaussian Processes

- A Gaussian Process is a collection of random variables that are jointly Gaussian and is fully characterized by its mean and covariance

$$
\begin{aligned}
f(\mathbf{x}) &\sim \mathcal{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}')) \\
m(\mathbf{x}) &= \mathbb{E}[f(\mathbf{x})] \\
k(\mathbf{x}, \mathbf{x}') &= \mathbb{E}[(f(\mathbf{x}) - m(\mathbf{x}))(f(\mathbf{x}') - m(\mathbf{x}'))]
\end{aligned}
$$

- example with two observations:

$$
\begin{aligned}
m(\mathbf{x}) &= 0 \\
k(\mathbf{x}, \mathbf{x}') &= \exp\left(-\frac{1}{2}(\mathbf{x} - \mathbf{x}')^T \Sigma (\mathbf{x} - \mathbf{x}')\right) \\
(y_1, y_2) &\sim \mathcal{N}(\mathbf{0}, K), \quad K = \begin{bmatrix} k(\mathbf{x}_1, \mathbf{x}_1), k(\mathbf{x}_1, \mathbf{x}_2) \\ k(\mathbf{x}_2, \mathbf{x}_1), k(\mathbf{x}_2, \mathbf{x}_2) \end{bmatrix}
\end{aligned}
$$

Training Gaussian Processes

- suppose we want to identify the model f in

$$y = f(\mathbf{x}) + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

- we observe n points from this model $\{\mathbf{x}_i, y_i\}_{i=1}^n$
- our goal is to identify μ, Σ and σ_n^2 such that

$$(y_1, y_2, \ldots, y_n) \sim \mathcal{N}(\mu, \Sigma + \sigma_n^2 I)$$

- we can parametrize the function f by

$$f(\mathbf{x}) \sim \mathcal{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}'))$$

- we optimize parameters θ in m, k and σ_n^2 by maximizing the log likelihood

$$\log(p(\mathbf{y} \mid X, \theta)) = -\frac{1}{2}\mathbf{y}^T (K + \sigma_n^2 I)^{-1}\mathbf{y} - \frac{1}{2}\log|K + \sigma_n^2 I| - \frac{n}{2}\log 2\pi$$

Prediction using Gaussian Processes

- once we optimize m, k and σ_n^2, we can predict on new observations $X_\star$

$$\begin{bmatrix}\mathbf{y}\\ \mathbf{y}_\star\end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix}m(X)\\ m(X_\star)\end{bmatrix}, \begin{bmatrix}K(X,X)+\sigma_n^2 I & K(X,X_\star)\\ K(X_\star,X) & K(X_\star,X_\star)\end{bmatrix}\right)$$

- $\mathbf{y}_\star|\mathbf{y}$ is normally distributed with mean and variance

$$\bar{\mathbf{y}}_\star = m(X_\star) + K(X_\star,X)\left(K+\sigma_n^2 I\right)^{-1}(\mathbf{y} - m(X_\star))$$
$$\sigma_{\mathbf{y}_\star}^2 = K(X_\star,X_\star) - K(X_\star,X)\left(K+\sigma_n^2 I\right)^{-1}K(X,X_\star)$$

Gaussian Process Model

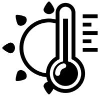
$$\underbrace{P_t}_{Y\in\mathbb{R}^n} = f_P(\underbrace{P_{t-l},\dots,P_{t-1},w_{t-m},\dots,w_t,u_{t-p},\dots,u_t}_{X\in\mathbb{R}^{n\times d}})$$

$$x_t = [P_{t-l},\dots,P_{t-1},w_{t-m},\dots,w_t,u_{t-p},\dots,u_t]$$

$$\begin{aligned}
P_t &\sim \mathcal{N}\left(\bar{P}_t,\sigma_t^2\right)\\
\bar{P}_t &= \mu(x_t) + K_\star K^{-1}(Y-\mu(X))\\
\sigma_t^2 &= K_{\star\star} - K_\star K^{-1} K_\star^T\\
K_\star &= [k(x_t,x_1),\dots,k(x_t,x_N)], K_{\star\star} = k(x_t,x_t)
\end{aligned}$$

Learning Problem

weather

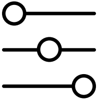


- outside temp. X^{d_1}
- outside humidity X^{d_2}
- solar radiation X^{d_3}

building

- power consumption Y
- internal gains X^{d_4}

control



- cooling temp. X^{c_1}
- supply air temp. X^{c_2}
- chilled water temp. X^{c_3}

The goal is to predict the zone temperature for multiple steps ahead

$$\begin{pmatrix} Y_{\mathrm{k+1}} \\ Y_{\mathrm{k+2}} \\ \vdots \\ Y_{\mathrm{k+N}} \end{pmatrix} = f(\overbrace{\underbrace{X^d_k, \dots, X^d_{k+N-1}}_{\text{disturbance}}, \underbrace{Y_{\mathrm{k}}, \dots, Y_{\mathrm{k}-\delta}}_{\text{autoregression}}}^{\text{non-manipulated variables}}, \overbrace{X^c_k, \dots, X^c_{k+N-1}}^{\text{control variables}})$$

Blackbox models

$$y_t = f(\overbrace{\underbrace{y_{t-l}, \ldots, y_{t-1}}_{\text{autoregression}}, \underbrace{w_{t-m}, \ldots, w_t}_{\text{disturbance}}}^{\text{non-manipulated variables}}, \overbrace{u_{t-p}, \ldots, u_t}^{\text{control variables}})$$

$$y_t = f(y_{t-l}, \ldots, y_{t-1}, w_{t-m}, \ldots, w_t, u_{t-p}, \ldots, u_t)$$

Blackbox models

$$P_t = f_P(P_{t-l}, \ldots, P_{t-1}, w_{t-m}, \ldots, w_t, u_{t-p}, \ldots, u_t)$$

$$T_t^i = f_T^i(T_{t-l'}, \ldots, T_{t-1}, w_{t-m'}, \ldots, w_t, u_{t-p'}, \ldots, u_t)$$
$$i \in \{1, \ldots, \text{number of zones}\}$$

$$\begin{aligned}
\underset{u_t, \ldots, u_{N-1}}{\text{minimize}} \quad & \sum_{t=0}^{N-1} (P_t - P_{\text{ref}})^2 \\
\text{subject to} \quad & P_t = f_P(P_{t-l}, \ldots, P_{t-1}, w_{t-m}, \ldots, w_t, u_{t-p}, \ldots, u_t) \\
& T_t^i = f_T^i(T_{t-l'}^i, \ldots, T_{t-1}^i, w_{t-m'}, \ldots, w_t, u_{t-p'}, \ldots, u_t) \\
& T_{\min} \leq T_t^i \leq T_{\max} \\
& u_{\min} \leq u_t \leq u_{\max} \\
& t \in \{0, \ldots, N-1\}
\end{aligned}$$

Why can't we use black-box models for control?

$$P_t = f(\overbrace{\underbrace{P_{t-l}, \dots, P_{t-1}}_{\text{autoregression}}, \underbrace{w_{t-m}, \dots, w_t}_{\text{disturbance}}}^{\text{non-manipulated variables}}, \overbrace{u_{t-p}, \dots, u_t}^{\text{control variables}})$$

$$\forall t = 1, \dots, N.$$

$$\begin{aligned}
\underset{u_t, \dots, u_{N-1}}{\text{minimize}} \quad & \sum_{t=0}^{N-1} (P_t - P_{\text{ref}})^2 \\
\text{subject to} \quad & P_t = f_P(P_{t-l}, \dots, P_{t-1}, w_{t-m}, \dots, w_t, u_{t-p}, \dots, u_t) \\
& T_t^i = f_T(T_{t-l'}^i, \dots, T_{t-1}^i, w_{t-m'}, \dots, w_t, u_{t-p'}, \dots, u_t) \\
& T_{\min} \le T_t^i \le T_{\max} \\
& u_{\min} \le u_t \le u_{\max} \\
& t \in \{0, \dots, N-1\}
\end{aligned}$$

Model Predictive Control

$$
\begin{aligned}
\underset{u_t,\ldots,u_{N-1}}{\text{minimize}} \quad & \sum_{\tau=0}^{N-1} (\bar{P}_{t+\tau} - P_{\text{ref}})^2 + \lambda \sigma^2_{P,t+\tau} \\
\text{subject to} \quad & \left.\begin{aligned} \bar{P}_{t+\tau} &= \mu(x_{t+\tau}) + K_\star K^{-1}(Y - \mu(X)) \\ \sigma^2_{P,t+\tau} &= K_{\star\star} - K_\star K^{-1} K_\star^T \end{aligned}\right\} \text{power model} \\
& \left.\begin{aligned} \bar{T}_{t+\tau} &= \mu(x_{t+\tau}) + K_\star K^{-1}(Y - \mu(X)) \\ \sigma^2_{T,t+\tau} &= K_{\star\star} - K_\star K^{-1} K_\star^T \end{aligned}\right\} \text{temperature model} \\
& u_{\min} \leq u_{t+\tau} \leq u_{\max} \\
& \tau \in \{0, \ldots, N-1\} \\
& \Pr(T_{\min} \leq T_{t+\tau} \leq T_{\max}) \geq 1 - \epsilon
\end{aligned}
$$

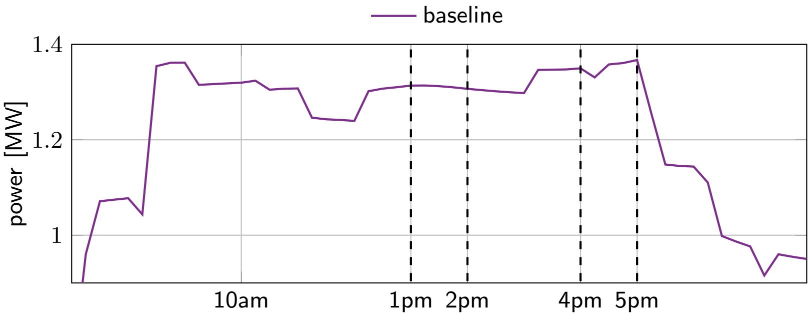
Data-driven MPC

$$
\begin{aligned}
\underset{u_t,\ldots,u_{N-1}}{\text{minimize}} \quad & \sum_{\tau=0}^{N-1} (\bar{P}_{t+\tau} - P_{\text{ref}})^2 + \lambda \sigma^2_{P,t+\tau} \\
\text{subject to} \quad & \left.\begin{aligned} \bar{P}_{t+\tau} &= \mu(x_{t+\tau}) + K_\star K^{-1}(Y - \mu(X)) \\ \sigma^2_{P,t+\tau} &= K_{\star\star} - K_\star K^{-1} K_\star^T \end{aligned}\right\} \text{power model} \\
& \left.\begin{aligned} \bar{T}_{t+\tau} &= \mu(x_{t+\tau}) + K_\star K^{-1}(Y - \mu(X)) \\ \sigma^2_{T,t+\tau} &= K_{\star\star} - K_\star K^{-1} K_\star^T \end{aligned}\right\} \text{temperature model} \\
& \Pr(T_{\min} \leq T_{t+\tau} \leq T_{\max}) \geq 1 - \epsilon \\
& u_{\min} \leq u_{t+\tau} \leq u_{\max} \\
& \tau \in \{0, \ldots, N-1\}
\end{aligned}
$$

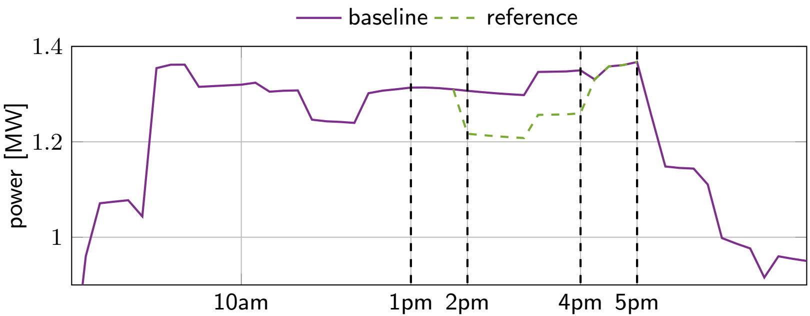
Physics-based MPC

$$
\begin{array}{ll}
\underset{u_t,\ldots,u_{N-1}}{\text{minimize}} & \sum_{\tau=0}^{N-1} (P_{t+\tau}(x_{t+\tau}) - P_{\text{ref}})^2 \\
\text{subject to} & x_{t+\tau} = Ax_{t+\tau-1} + Bu_{t+\tau-1} + B_w w_{t+\tau-1} \\
& B = B_u + B_{xu}[x_{t+\tau-1}] + B_{wu}[w_{t+\tau-1}] \\
& T_{\min} \leq T_{t+\tau}(x_{t+\tau}) \leq T_{\max} \\
& u_{\min} \leq u_{t+\tau} \leq u_{\max} \\
& \tau \in \{0, \ldots, N-1\}
\end{array}
$$

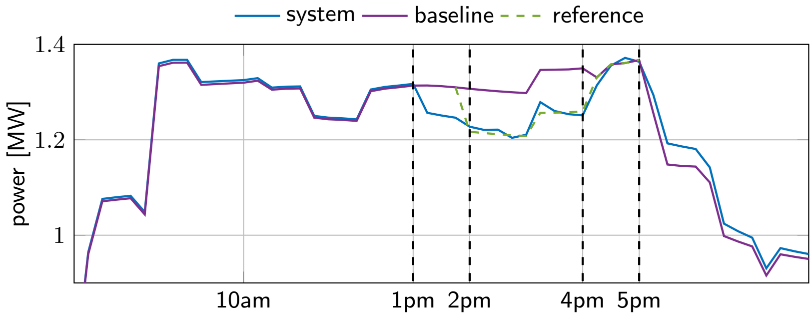
OED Example



OED Example

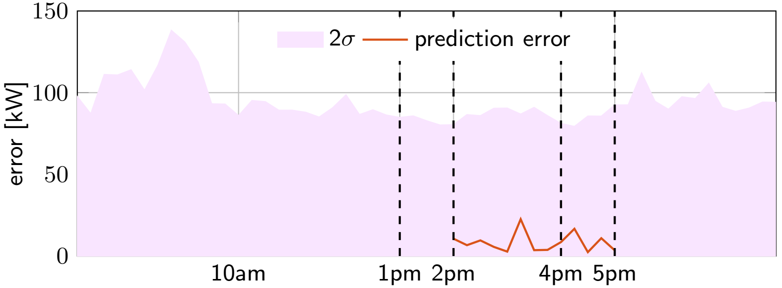


OED Example



system
baseline
reference
power [MW]
1.4
1.2
1
10am
1pm
2pm
4pm
5pm

OED Example



Optimal Experiment Design

Goal

Learn the hyperparameters θ in $y \sim \mathcal{GP}(m(x), k(x); \theta)$ as fast as possible as we add new samples.

Formal Definition

$$H(\theta|\mathcal{D}) = -\int p(\theta|\mathcal{D}) \log(p(\theta|\mathcal{D}))d\theta$$

$$\arg\max_x H(\theta|\mathcal{D}) - \mathbb{E}_{y\sim\mathcal{N}\left(\bar{y}(x),\sigma^2(x)\right)} H(\theta|\mathcal{D}, x, y)$$

Equivalent Definition

$$\arg\max_x H(y|x,\mathcal{D}) - \mathbb{E}_{\theta\sim p(\theta|\mathcal{D})} H(y|x,\theta)$$

using $H(\theta) - H(\theta|y) = H(y) - H(y|\theta)$, and

$$p(y|x,\mathcal{D}) = \int p(y|x,\theta,\mathcal{D})p(\theta|\mathcal{D})d\theta \approx \mathcal{N}\left(\tilde{y}(x), \tilde{\sigma}^2(x)\right)$$

Optimal Experiment Design

Goal

Learn the hyperparameters θ in $y \sim \mathcal{GP}(m(x), k(x); \theta)$ as fast as possible as we add new samples.

Equivalent Definition

$$\arg\max_x H(y|x, \mathcal{D}) - \mathbb{E}_{\theta\sim p(\theta|\mathcal{D})} H(y|x, \theta)$$

using $H(\theta) - H(\theta|y) = H(y) - H(y|\theta),$ and

$$p(y|x, \mathcal{D}) = \int p(y|x, \theta, \mathcal{D}) p(\theta|\mathcal{D}) d\theta \approx \mathcal{N}\left(\tilde{y}(x), \tilde{\sigma}^2(x)\right)$$

Sequential sampling for OED

$$\begin{aligned} \underset{u_t}{\text{maximize}} \quad & \tilde{\sigma}^2(x_t)/\sigma^2(x_t) \\ \text{subject to} \quad & x_t = [y_{t-l}, \ldots, y_{t-1}, u_{t-m}, \ldots, u_t, w_{t-p}, \ldots, w_t] \\ & u_t \in \mathcal{U} \end{aligned}$$

OED + Evolving Gaussian Processes

Sequential sampling for OED

$$\begin{aligned} \underset{x}{\text{maximize}} \quad & \text{information gain / variance}(x) \\ \text{subject to} \quad & \text{operation constraints}(x) \end{aligned}$$

Optimal subset of data selection

$$\underset{x_j \mid (x_j, y_j) \in \mathcal{D} \setminus \mathcal{S}}{\text{maximize}} \quad \text{information gain / variance}(x)$$

Sequential sampling for OED based on Information Gain

Initialization

if initial $\mathcal{D} := (X, Y)$ **then**
Compute $\theta_{\mathrm{MLE}} = \arg\max_{\theta^{\mathrm{MLE}}} \Pr(Y|X, \theta)$
Assign priors $\theta_0 \sim \mathcal{N}\left(\theta_{\mathrm{MLE}}, \sigma^2_{\mathrm{init}}\right)$
else
Assign priors $\theta_0 \sim \mathcal{N}\left(\mu_{\mathrm{init}}, \sigma^2_{\mathrm{init}}\right)$
end if

Sampling

while $t < t_{\max}$ **do**
Calculate features x_t in (**??**) as a function of u_t
Solve (**??**) to calculate optimal u_t^*
Apply u_t^* to the system and measure y_t
$\mathcal{D} = \mathcal{D} \cup (x_t, y_t)$
Update $\theta_{\mathrm{t}} = \arg\max_{\theta^{\mathrm{MAP}}} \Pr(Y|X, \theta_{\mathrm{t}-1})$
end while

Optimization for Sequential Experiment Design

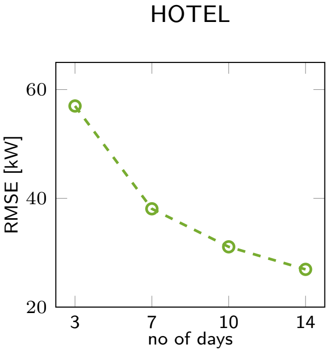
$$\begin{aligned}
\text{maximize}_{\mathbf{u_t}} \quad & \text{information gain}(x_t) \\
\text{subject to} \quad & x_t = [P_{t-l}, \ldots, P_{t-1}, w_{t-m}, \ldots, w_t, u_{t-p}, \ldots, \mathbf{u_t}] \\
& 22^\circ\mathrm{C} \leq \text{cooling set-point} \leq 27^\circ\mathrm{C}, \\
& 12^\circ\mathrm{C} \leq \text{supply air set-point} \leq 14^\circ\mathrm{C}, \\
& 3.7^\circ\mathrm{C} \leq \text{chilled water set-point} \leq 9.7^\circ\mathrm{C}, \\
& \text{rate of change in chilled water set-point} \leq 2^\circ\mathrm{C}/15\mathrm{min}.
\end{aligned}$$

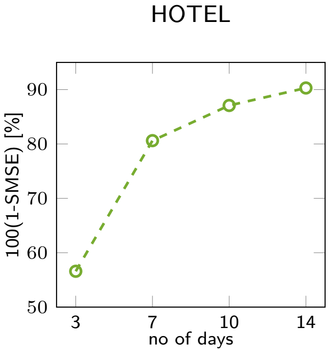
Evolving Gaussian Processes

Optimal subset of data selection

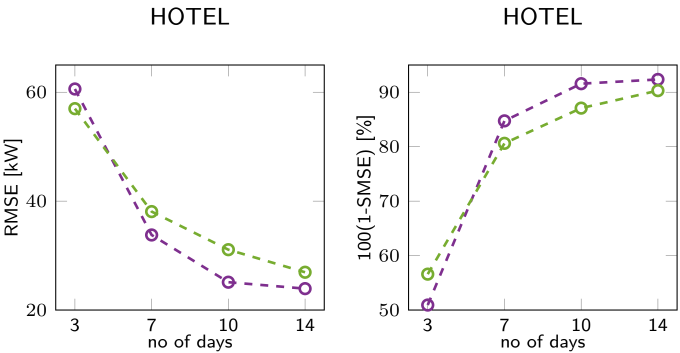
$$\underset{x_j \mid (x_j, y_j) \in \mathcal{D} \setminus \mathcal{S}}{\text{maximize}} \quad \tilde{\sigma}^2(x_j) / \sigma^2(x_j)$$

OED Example


HOTEL
RMSE [kW]
60
40
20
3
7
10
14
no of days


HOTEL
100(1-SMSE) [%]
90
80
70
60
50
3
7
10
14
no of days

OED Example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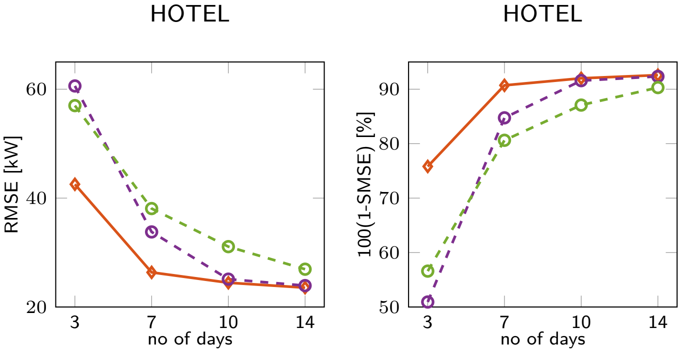
no of days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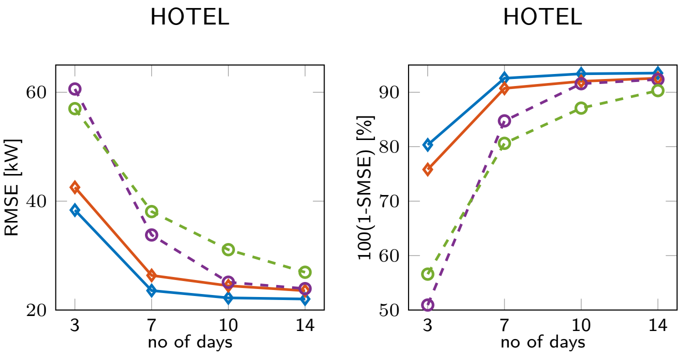
HOTEL
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90
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no of days