Towards a Turnkey Model Predictive Controller: Identification, Application, and Theory

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Turnkey MPC

- 2 Identification of integrating disturbance models
- 3 Combined identification and offset-free control
- Stability of offset-free MPC

Outline

Turnkey MPC

- Process control and turnkey
- The power of integrators
- Offset-free model predictive control

2 Identification of integrating disturbance models

3 Combined identification and offset-free control

4 Stability of offset-free MPC

- Process control: active regulation of industrial systems (chemical plants, power systems, building energy systems, etc.).
- Broad goal: **profitably** maintain operating conditions while satisfying **safety**, **environmental**, and quality constraints.
- To meet industry demands, it is necessary to design process operations in a way that is rigorous and data-driven.



Process control hierarchy. Dashed box: model-based problems. Adapted from Seborg, Edgar, Mellichamp, and Doyle (2017).

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Process control hierarchy. Dashed box: model-based problems. Adapted from Seborg et al. (2017).



Controller: based on measurements, choose the inputs that reconciles plant behavior with the reference signal, **AND** attenuate or correct for the effect of disturbances.

¹Fractionating columns, used in petroleum and petrochemical production

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The basic reference tracking problem



Controller: based on measurements, choose the inputs that reconciles plant behavior with the reference signal, **AND** attenuate or correct for the effect of disturbances.

²Crazyflie 2.0 quadcopter platform for research and education (Giernacki, Skwierczyński, Witwicki, Wroński, and Kozierski, 2017).

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³Temperature Control Laboratory (TCLab) Arduino platform for research and education (Park, Martin, Kelly, and Hedengren, 2020).

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Observer problem: find a state sequence that minimizes the magnitude of the noise sequences implied by **past** measurements and inputs.

Regulator problem: find the **future input sequence** that minimizes distance from the reference signal based on the current state estimate.

To close the loop, implement the first input from the regulator solution, and move to the next sample time.



• **Turnkey MPC**: automated application of MPC to a process, from tuning of the components, to monitoring the closed-loop system.

• All of these are well-studied problems. Why isn't there a turnkey solution to MPC in process industries?

• Gaps in the literature remain wherever integrators are used in MPC.



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- **Turnkey MPC**: automated application of MPC to a process, from tuning of the components, to monitoring the closed-loop system.
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- Gaps in the literature remain wherever integrators are used in MPC.

- In classical control, the bane of proportional-only control is the steady-state error.
- For example, the response of P vs PI control to an unmeasured disturbance:



• We have similar behavior for the response to a setpoint under plant-model mismatch:





Figure: Adapted from Rawlings, Mayne, and Diehl (2020).

- MPC has similar problems, only converging to the setpoint in the absence of unmeasured disturbances, and without plant-model mismatch.
- Offset-free MPC rejects disturbances and corrects for mismatch.
- In offset-free MPC, we add integrators directly into the model as "integrating disturbances":

$$x^{+} = Ax + B_{d}d + Bu + w$$
$$d^{+} = d + w_{d}$$
$$y = Cx + C_{d}d + v$$

where (w, w_d, v) are noise terms.

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Figure: Adapted from Rawlings, Mayne, and Diehl (2020).

- State-space summary of model predictive control:
 - ► Observer: where are we?
 - ► Target selector: where should we go?
 - Regulator: how do we get there?
- Standard MPC: persistent disturbances ⇒ persistent offset (from the reference)!
- Offset-free MPC model the disturbances as integrators. Same function as the "I" in PI control.



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Outline

Turnkey MPC

- 2 Identification of integrating disturbance models
 - Observer "tuning"
 - Augmenting standard models with integrating disturbances
 - Direct maximum likelihood identification

3 Combined identification and offset-free control

4 Stability of offset-free MPC

Linear augmented disturbance model

$$\begin{bmatrix} x \\ d \end{bmatrix}^{+} = \begin{bmatrix} A & B_d \\ 0 & I \end{bmatrix} \begin{bmatrix} x \\ d \end{bmatrix} + \begin{bmatrix} B \\ 0 \end{bmatrix} u + \begin{bmatrix} w \\ w_d \end{bmatrix} \begin{bmatrix} w \\ w_d \\ v \end{bmatrix} \stackrel{\text{iid}}{\sim} N(0, S_d)$$

$$y = \begin{bmatrix} C & C_d \end{bmatrix} \begin{bmatrix} x \\ d \end{bmatrix} + v$$

Steady-state Kalman filter
$$\begin{bmatrix} \hat{x} \\ \hat{d} \end{bmatrix}^{+} = \begin{bmatrix} A & B_{d} \\ 0 & I \end{bmatrix} \begin{bmatrix} \hat{x} \\ \hat{d} \end{bmatrix} + \begin{bmatrix} B \\ 0 \end{bmatrix} u \\ + \begin{bmatrix} K_{x} \\ K_{d} \end{bmatrix} \begin{pmatrix} y - \begin{bmatrix} C & C_{d} \end{bmatrix} \begin{bmatrix} \hat{x} \\ \hat{d} \end{bmatrix} \end{pmatrix}$$

 \Rightarrow

Noise covariance matrix $S_d \Rightarrow Observer gains \begin{bmatrix} K_x \\ K_d \end{bmatrix}$



- We cannot do optimal state estimation because our model is *not general*,
- **but**, since S_d is diagonal, we only have to tune $n + n_d + n_y$ variance parameters.

General disturbance model



- General model \Rightarrow we can get optimal state estimation!
- Two options: (1) tune $(n + n_d + n_y)^2$ variance parameters and check positive definiteness, or (2) fit S_d from data.¹

¹Kuntz and Rawlings (2022a,b); Kuntz, Downs, Miller, and Rawlings (2023a,b,c); Kuntz and Rawlings (2024)

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First solution: augment standard (closed-form) ID methods with an integrating disturbance model.



$$\begin{aligned} x^{+} &= Ax + B_{d}d + Bu + w \\ d^{+} &= d + w_{d} \\ y &= Cx + C_{d}d + v \\ w_{d} \\ v \\ \end{bmatrix}^{\text{iid}} \mathrm{N}(\mathbf{0}, S_{d}) \end{aligned}$$

¹Larimore (1990); Verhaegen (1994)

²Theorem 8.2.1 in Anderson (2003)

³Muske and Badgwell (2002); Pannocchia and Rawlings (2003)

⁴Kuntz and Rawlings (2022a,b); Kuntz et al. (2023a,b)

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Maximum likelihood estimation of disturbance models

First solution: augment standard (closed-form) ID methods with an integrating disturbance model.



 $x^{+} = Ax + B_{d}d + Bu + w$ $d^{+} = d + w_{d}$ $y = Cx + C_{d}d + v$ $\begin{bmatrix} w \\ w_{d} \\ v \end{bmatrix} \stackrel{\text{iid}}{\sim} N(0, S_{d})$

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TCLab: a benchmark temperature control laboratory



- Two heaters, two temperature sensors.
- Fully observed states, output disturbance model:

$$x^+ = Ax + Bu + w,$$
 $d^+ = d + w_d,$ $y = x + d + v$

- ID: use ARX methods to find (A, B) matrices, then augment with a noise model.
- Offset-free control: test with setpoint changes.

First, we identify the plant and disturbance models.



Next, the identified ARX model is used to design an offset-free MPC and track setpoints.



Maximum likelihood identification with integrating disturbance models

• Subsume disturbance into state $\tilde{x}_k \leftarrow \begin{bmatrix} x_k \\ d_k \end{bmatrix}$ and re-write in Kalman innovation form:

Linear augmented disturbance model $\begin{bmatrix} x \\ d \end{bmatrix}^{+} = \begin{bmatrix} A & B_{d} \\ 0 & I \end{bmatrix} \begin{bmatrix} x \\ d \end{bmatrix} + \begin{bmatrix} B \\ 0 \end{bmatrix} u + \begin{bmatrix} w \\ w_{d} \end{bmatrix} \qquad \begin{bmatrix} w \\ w_{d} \\ v \end{bmatrix} \stackrel{\text{iid}}{\sim} N(0, S_{d}) \Rightarrow$ $y = \begin{bmatrix} C & C_{d} \end{bmatrix} \begin{bmatrix} x \\ d \end{bmatrix} + v$

Parameterized Kalman filter $\tilde{x}^+ = A(\theta)\tilde{x} + B(\theta)u + K(\theta)e$ $e := y - C(\theta)\tilde{x} \stackrel{\text{iid}}{\sim} N(0, R_e(\theta))$

where R_e is the innovation error and K is the steady-state Kalman gain matrix.

• Maximum likelihood: maximize, over the parameters, the probability of observing the data we have collected.

$$\min_{ heta}\left(-\ln p(\mathbf{y}_{N-1}|\mathbf{u}_{N-1}, heta)
ight) \propto rac{N}{2}\ln\det R_{e}(heta) + rac{1}{2}\sum_{k=0}^{N-1}\left|y_{k}-\hat{y}_{k}(heta)
ight|_{[R_{e}(heta)]^{-1}}^{2}$$

• Looks great! What could go wrong?

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$$\min_{\theta} \left(-\ln p(\mathbf{y}_{N-1}|\mathbf{u}_{N-1},\theta)\right) \propto \frac{N}{2} \ln \det R_e(\theta) + \frac{1}{2} \sum_{k=0}^{N-1} |y_k - \hat{y}_k(\theta)|^2_{[R_e(\theta)]^{-1}}$$

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• Looks great! What could go wrong?

Same as before: identify the plant and disturbance models. This time, ARX vs ML.



Standard ML identification: what could go wrong? (cont.)

Use each model to design an offset-free MPC and track setpoints.



This time, ML model goes unstable! (Turns off.) What went wrong?

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Constrained/regularized maximum likelihood identification

• What went wrong? ML identification (asymptotically) minimizes the distance (in relative entropy) between the data and model:

$$\hat{ heta}_{N}pprox rgmin_{ heta} N^{-1}\mathbb{E}[\ln p(\mathbf{y}_{N-1}|\mathbf{u}_{N-1}, heta)]$$

Without plant-model mismatch, estimates inherit plant properties!

- With integrating disturbances, ML identification may estimate an unstable Kalman filter!
- Regularized maximum likelihood:

$$\min_{\theta} \frac{N}{2} \ln \det R_e(\theta) + \frac{1}{2} \sum_{k=0}^{N-1} |y_k - \hat{y}_k(\theta)|^2_{[R_e(\theta)]^{-1}} + \rho |\theta - \theta_0|^2$$

• Constrained maximum likelihood:

$$\min_{\theta} \frac{N}{2} \ln \det R_{e}(\theta) + \frac{1}{2} \sum_{k=0}^{N-1} |y_{k} - \hat{y}_{k}(\theta)|^{2}_{[R_{e}(\theta)]^{-1}} \text{ subject to } A(\theta) - K(\theta)C(\theta) \text{ stable}$$

• Eigenvalue constraints are nondifferentiable, so we: (1) convert to differentiable semidefinite matrix inequalities (nonlinear SDP) and (2) get rid of semidefinite arguments/constraints with Cholesky factorization algorithm (Kuntz and Rawlings, 2024).

Constrained/regularized maximum likelihood identification

• What went wrong? ML identification (asymptotically) minimizes the distance (in relative entropy) between the data and model:

$$\hat{\theta}_N \approx \operatorname*{argmin}_{\theta} N^{-1} \mathbb{E}[\ln p(\mathbf{y}_{N-1} | \mathbf{u}_{N-1}, \theta)]$$

Without plant-model mismatch, estimates inherit plant properties!

- With integrating disturbances, ML identification may estimate an unstable Kalman filter!
- **Regularized** maximum likelihood:

$$\min_{\theta} \frac{N}{2} \ln \det R_e(\theta) + \frac{1}{2} \sum_{k=0}^{N-1} |y_k - \hat{y}_k(\theta)|^2_{[R_e(\theta)]^{-1}} + \rho |\theta - \theta_0|^2 \right]$$

• Constrained maximum likelihood:

$$\min_{\theta} \frac{N}{2} \ln \det R_e(\theta) + \frac{1}{2} \sum_{k=0}^{N-1} |y_k - \hat{y}_k(\theta)|^2_{[R_e(\theta)]^{-1}} \text{ subject to } A(\theta) - K(\theta)C(\theta) \text{ stable}$$

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Turnkey MPC

Identification of integrating disturbance models

3 Combined identification and offset-free control

- Temperature control laboratory
- Eastman case study

Stability of offset-free MPC





- Same data as before.
- Same model as before (except Augmented PCA, which is taken from Kuntz and Rawlings (2022a)):

$$x^+ = Ax + Bu + w,$$
 $d^+ = d + w_d,$ $y = x + d + v$

Fitting a wider range of ML models:



Closed-loop comparison of all models' offset-free MPC designs:



Comparing time-averaged tracking performance $\ell := |y - y_{sp}|^2$ and estimation performance $e^{\top}e$:



Constrained maximum likelihood models are as good or better than the previous models.

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Figure: Schematic of the DMT reactor and MPC control strategy.

 Reactor produces DMT via TPA methylation:¹

 $TPA + 2MeOH \Longrightarrow DMT + 2H_2O$

• Goal: replace the >20 year old, hand-tuned MPC implementation by re-identifying (in the closed-loop) the plant and disturbance model in > 1 day.

 $^{^{1}}$ DMT = dimethyl terephthalate, TPA = terephthalic acid.



- System excited with setpoint changes while previous MPC is running; some setpoints not reached!
- New model predicts long-term behavior better than previous model. Possibly explains previous failure to reach setpoints.

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Eastman application: closed-loop re-identification



- System excited with setpoint changes while previous MPC is running; some setpoints not reached!
- Newly fitted model correctly predicts more long-term behavior than previous model. Possibly explains failure to reach setpoints.

Eastman application: before and after experiment



- The performance indicators $(\ell := |Hy r_{sp}|^2_{Q_y}, Q_y := \text{diag}(10^{-4}, 1, 10^{-3}), H := \begin{bmatrix} I_3 & 0 \end{bmatrix})$ substantially favor the new model.
- Time-averaged tracking error is substantially lower (38%) with the new model.
- The entire distribution of stage costs is shifted to smaller values.

1 Turnkey MPC

2 Identification of integrating disturbance models

3) Combined identification and offset-free control

Stability of offset-free MPC

- Robust vs offset-free performance
- Simple pendulum
- Continuous stirred-tank reactor

• **Robust performance**: we exceed nominal costs *continuously* with disturbance magnitude.

• Offset-free performance: we regain nominal stability if the setpoints/disturbances are *asymptotically constant*; otherwise, the setpoint tracking is robust to the setpoint/disturbance *increments*.



While the robust stability properties of MPC are well-known, there are no *stability* results on the offset-free property for nonlinear MPC with integrating disturbances.

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- Offset-free MPC theorems typically assume a steady state is reached and then prove that the steady state must achieve the setpoints.
- Tracking MPC theorems can prove convergence to setpoints, but they must assume a priori knowledge of the plant dynamics because an integrating disturbance is not used.
- Problem statement:

$$\begin{aligned} x_{\rm P}^+ &= f_{\rm P}(x_{\rm P}, u, w_{\rm P}), & y &= h_{\rm P}(x_{\rm P}, u, w_{\rm P}), & r &= g(u, y) & ({\rm plant}) \\ x^+ &= f(x, u, d), & y &= h(x, u, d), & r &= g(u, y) & ({\rm model}) \\ f(x, u, 0) &= f_{\rm P}(x, u, 0), & h(x, u, 0) &= h_{\rm P}(x, u, 0) & ({\rm nominal \ consistency}) \end{aligned}$$

• Want to show offset-free MPC is a controller for which

 $(w_{\mathrm{P}}(k), r_{\mathrm{sp}}(k)) \to (w_{\infty}, r_{\infty}) \qquad \mathrm{implies} \qquad r(k) - r_{\mathrm{sp}}(k) \to 0$

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Simple pendulum

$$\dot{x} = \begin{bmatrix} \text{Plant:} \\ x_2 \\ \sin x_1 - (w_{\rm P})_1^2 x_2 + (5 + (w_{\rm P})_2)u + (w_{\rm P})_3 \end{bmatrix}.$$

Model:
$$x^+ = x + 0.1 \begin{bmatrix} x_2 \\ \sin x_1 + 5u \end{bmatrix}$$
.



Simple pendulum

Plant:
$$\dot{x} = \begin{bmatrix} x_2 \\ \sin x_1 - x_2 + 7u + 3H(t - 14) \end{bmatrix}$$
.

Model:
$$x^+ = x + 0.1 \begin{bmatrix} x_2 \\ \sin x_1 + 5u \end{bmatrix}$$
.



Simple pendulum: swing upright

Plant:
$$\dot{x} = \begin{bmatrix} x_2 \\ \sin x_1 - x_2 + 7u + 3H(t - 14) \end{bmatrix}$$

Model:
$$x^+ = x + 0.1 \begin{bmatrix} x_2 \\ \sin x_1 + 5u \end{bmatrix}$$
.

MPC with no disturbance model:

- successful swing up,
- unsuccessful half-way balance, and
- unsuccessful disturbance rejection.

The nominal MPC problem is:

$$\min_{\mathbf{x} \in (\mathbb{R}^n)^{N+1}, \mathbf{u} \in \mathbb{U}^N} |x(N)|_{P_f}^2 + \sum_{k=0}^{N-1} |x(k)|_Q^2 + |u(k)|_R^2 \qquad \text{subject to} \qquad \begin{array}{l} x(0) = x, \\ x(k+1) = f(x(k), u(k), 0), \\ |x(N)|_{P_f}^2 \le c_f. \end{array}$$

Denote the solutions by $u^0(k; x)$ and $x^0(k; x)$ and let $\kappa_N(x) := u^0(0; x)$.

Theorem (Stability of MPC despite plant-model mismatch)

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- the standard inherent robustness assumptions¹ hold,
- Ithe stage and terminal costs are positive definite quadratics,
- the dynamics are differentiable,
- **9** and the origin is a steady state uniformly in the disturbance $w_{\rm P}$,

then there exists $\delta > 0$ such that the closed-loop system $x^+ = f_P(x, \kappa_N(x), w_P), |w_P| \le \delta$ is exponentially stable.²

¹Assumptions 1–4 from Allan, Bates, Risbeck, and Rawlings (2017) were used.

Simple pendulum: offset-free control

Plant:
$$\dot{x} = \begin{bmatrix} x_2 \\ \sin x_1 - x_2 + 7u + 3H(t - 14) \end{bmatrix}$$

Model:
$$x^+ = x + 0.1 \begin{bmatrix} x_2 \\ \sin x_1 + 5u + d \end{bmatrix}$$
.

- Offset-free MPC vs MPC with no disturbance model:
 - both successfully swing up,
 - only offset-free MPC successfully does the half-way balance, and
 - only offset-free MPC successfully rejects the disturbance.

Nonisothermal CSTR

Plant: $\dot{x} = \begin{bmatrix} \frac{0.95 - x_1}{20} - ke^{-5.05/x_2} x_1\\ \frac{0.39 - x_2}{20} + ke^{-5.05/x_2} x_1 - 0.12u(x_2 - 0.38 + \frac{H(t - 300)}{20}) \end{bmatrix}$ Model: $x^{+} = x + \left[\frac{\frac{1 - x_{1}}{20} - ke^{-5/x_{2}}x_{1}}{\frac{0.39 - x_{2}}{20} + ke^{-5/x_{2}}x_{1} - 0.12u(x_{2} - 0.38 - d)} \right]$ 1.0 $x(\mathbf{0})$





Nonisothermal CSTR: no mismatch



Nonisothermal CSTR: with mismatch



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Turnkey MPC

Nonisothermal CSTR: torture test



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Turnkey MPC

Nonisothermal CSTR: torture test



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Turnkey MPC

Theorem (Stability of offset-free MPC)

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- the steady-state targets (x_s, u_s) are Lipschitz continuous in (r_{sp}, d) ,
- the plant and model are observable at each steady state,
- **③** the standard inherent robustness assumptions¹ hold uniformly in (r_{sp}, d) ,
- the stage and terminal costs are quadratics with weights $Q, R, P_f(r_{sp}, d)$,
- Ithe plant and model dynamics are differentiable,
- the estimator is robustly globally exponentially stable (uniformly in u), then there exist $\delta, \delta_w > 0$ such that

 $|(\Delta r_{\rm sp}(k), \Delta w_{\rm P}(k))| \to 0$ implies $|r(k) - r_{\rm sp}(k)| \to 0$

so long as $|(\Delta r_{\rm sp}, \Delta w_{\rm P})| \leq \delta$ and $|w_{\rm P}| \leq \delta_w$ at all times, where $\Delta r_{\rm sp}(k) := r_{\rm sp}(k) - r_{\rm sp}(k-1)$ and $\Delta w_{\rm P}(k) := w_{\rm P}(k) - w_{\rm P}(k-1)$.

- Identification: both rigorous and easy-to-implement algorithms for disturbance model identification.
- Application: in three days, we produced and validated a controller with 38% lower setpoint tracking error than a controller that was tuned and validated for >20 years!
- Theory: First-of-their-kind stability results for nonlinear offset-free model predictive control.



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