

Using Probabilistic Forecasts in Stochastic Optimization

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Abstract—In the coming years, the energy system will be transformed from central carbon-based power plants to decentralized renewable generation. Due to the dependency of these systems on external influences such as the weather, forecast uncertainties pose a problem. In this paper, we will compare different methods that mitigate the impact of these forecast uncertainties. Our results suggest that estimating these uncertainties and modeling them for optimization can increase the benefit for the individual system.

Index Terms—Stochastic Dynamic Programming, Model Predictive Control, Probabilistic PV Forecasting, Probabilistic Load Forecasting, PV Battery Systems

I. INTRODUCTION

In order to decrease CO₂ emissions and transition to a more sustainable future in the energy sector, an increased penetration of renewable generation into the electricity grid is necessary. Typically, the generation profile of renewable energy sources is dependent on external factors such as the weather, therefore, unlike conventional carbon-based power plants, production cannot be controlled. This introduces uncertainty into the system.

Another problem arises as electricity generation shifts from large centralized plants to a more decentralized system. In Germany, over 98% of all photovoltaic generators feed into low voltage distribution grids [1]. With less large power plants, the increased variability of the generation must be mitigated by the decentralized plants. To this end, the installment of storages is often incentivized. Optimal operation of these systems entails maximizing both individual benefit for the owner and minimizing negative impact on the electricity grid. This can be achieved by using predictive control strategies.

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However, the performance of these strategies largely depends on the accuracy of external forecasts for the generation profile as well as for possible uncontrollable loads in the system.

A. Existing Control Approaches

Various studies have been published which present methods of mitigating forecast uncertainties in the control of energy systems, most of the strategies presented in the literature are based on model predictive control (MPC). These strategies can be categorized into three groups

- In **Deterministic MPC**, state feedback is obtained via reoptimization at every timestep. Knowledge of the future is represented by a deterministic forecast. An update of the forecast with most recent measurements can be performed to mitigate uncertainties. Various studies have been published using this approach in different applications and different focuses [2]–[8].
- In **Scenario-based MPC** or two-stage stochastic MPC forecast uncertainty is considered by using scenario forecasts instead of deterministic ones. At each sampling time, the current control input is determined by minimizing the most probable costs and the recourse costs approximated with the scenario forecast. Studies discussing this approach can be found in [9]–[12].
- **Multi-stage Stochastic MPC** accounts for the fact that future state feedback depends on the realizations of the uncertain parameters and therefore the entire evolution of the system up to that point. This approach is implemented in [13]–[16] for linear systems. For nonlinear systems and relationships between uncertain parameter and control input dynamic programming can be used if the system has a low dimensionality [17]–[19].

Different methods for mitigating the uncertainty of forecasts for external influences have been studied. However, there is a distinct scarcity of studies comparing these methods in order to determine their suitability for certain application. In this

paper we will compare different methods of mitigating forecast uncertainties in optimal operation. Furthermore, we will study the impact a precise characterization of the forecast uncertainty could have on the system performance.

II. OPTIMIZATION UNDER UNCERTAINTY

A. Plant Model

We intend to control a system of a photovoltaic (PV) power generator combined with a storage system and an uncontrollable load. We use a generic description fitting to various applications such as PV battery systems, PV heatpump systems or photovoltaic charging of battery electric vehicles. We assume that the controlled plant can be completely described by a single state variable; the state of charge of the storage system x_k . A discrete time formulation with discretization timestep Δt and time index k is assumed. Furthermore, a single control variable u_k is used, denoting the power used to charge and discharge the storage. A stochastic external influence through PV production p_k^{PV} and household load p_k^{Load} on site is summarized by the variable

$$R_k = p_k^{\text{PV}} - p_k^{\text{Load}}. \quad (1)$$

Positive values for u_k and R_k denote the provisioning of energy into the common household bus i.e. discharging the battery and PV production exceeding the household load respectively.

The state transition of x_k is given by

$$x_{k+1} = f_k^x(x_k, u_k, R_k) \quad (2)$$

where the transition may only depend on the control, state, and residual generation state variable at the respective timestep. For simplicity, the state transition is assumed to be deterministic. Depending on the control paradigm, extension to a stochastic state transition may be possible. The allowed region of the state variable is denoted by \mathcal{X}

$$x_k \in \mathcal{X} \equiv \{x' | x^{\min} \leq x' \leq x^{\max}\} \quad \forall k \quad (3)$$

Typically, the state of charge is allowed between 0 and 1. However, a smaller interval is also possible to cater for increased storage aging or storage losses in low and high state of charge regions.

A constraint is set on the control variable as well

$$u_k \in \mathcal{P}(x_k) \quad \forall k, \quad (4)$$

where the set \mathcal{P} is not necessarily continuous.

B. Stochastic Optimization Problem

The system performance measurement J is described by stage costs and terminal costs

$$J = \sum_{k=0}^{N-1} g_k(x_k, u_k, R_k) + g_N(x_N, R_N) \quad (5)$$

where $g_k(x_k, u_k, R_k)$ denotes stage costs typically resulting from regulations or energy prices. The terminal costs

$g_N(x_N, R_N)$ account for energy in the storage at the end of the optimization horizon N .

Our goal is to find a set of control inputs $\mathbf{u} = [u_0, \dots, u_{N-1}]$ which control the system in a way that minimizes the overall costs of operation. However, J depends on the uncertain residual generation. This leads to a stochastic optimal control problem which reads

$$\min_{\mathbf{x}, \mathbf{u}} \mathbb{E}(J(\mathbf{x}, \mathbf{u}, \mathbf{R})) \quad (6)$$

subject to

$$\begin{aligned} x_{k+1} &= f^x(x_k, u_k) & \forall k = 0 \dots N-1 \\ x_k \in \mathcal{X} \quad u_k \in \mathcal{P}(x_k) & & \forall k = 0 \dots N \\ x_0 &= x_{\text{init}} \end{aligned}$$

where a boldface setting of a variable name denotes the timeseries over the complete horizon. In (6) the control input (and therefore also state) at timestep k may depend on the realization of R_i for $i \leq k$. Hence, u must be understood as a policy which defines a decision rule for the control dependent on x and R . However, this leads to an intractable optimization problem in the infinite dimensional state of policies. In the following, different methods to transform this problem into a tractable formulation will be presented.

C. Ensemble Forecast

As discussed, \mathbf{R} is a timeseries of an uncertain variable that can be modeled as a random distribution. Ensemble forecasts are used to estimate this distribution and approximate the expectation value in problem (6).

A forecast ensemble is a set of M possible trajectories of the residual generation each with a horizon length of N . The member m -th at timestep k is denoted by

$$\bar{R}_k^m. \quad (7)$$

The full ensemble forecast is denoted by $\bar{\mathbf{R}}$ and the mean forecast at timestep k with \hat{R}_k . The ensemble forecast for the residual generation is obtained by pairwise adding the members of individual forecast ensembles for load and photovoltaic generation.

$$\bar{R}_k^m = \bar{p}_{\text{PV}}^{m_{\text{PV}}} - \bar{p}_{\text{Load}}^{m_{\text{Load}}}, \quad (8)$$

where $\bar{p}_{\text{PV}}^{m_{\text{PV}}}$ denotes the m_{PV} -th of M_{PV} members of the PV ensemble and $\bar{p}_{\text{Load}}^{m_{\text{Load}}}$ denotes the m_{Load} -th of M_{Load} members of the load ensemble. This results in $M = M_{\text{PV}} \cdot M_{\text{Load}}$ members for the residual generation.

1) *PV Forecast Ensemble*: For the PV forecast we use the ensemble forecast from the Integrated Forecasting System of the European Centre for Medium-Range Weather Forecasts (ECMWF-IFS) which is upsampled to a time resolution of 15 min. We are considering the day ahead prediction of the 0:00 run of the model. PV generation is calculated using a parametric PV simulation for a PV plant in Freiburg, Germany with an azimuth angle of 17° and a declination of 30° .

Since the ECMWF ensemble $\bar{p}_{\text{PV}}^{m, \text{uncalib}}$ is underdispersive, we apply a variance deficit calibration to yield a forecast ensemble with an appropriate spread. For each forecast, this

calibration is done using the forecast and measurement data over the timespan of one month directly prior to the forecast. The root mean squared error (RMSE) of the mean forecast is calculated for that data. It is used to compute the variance deficit factor

$$\kappa_{\text{PV}}^{\text{VD}} = \frac{\text{RMSE}_{\text{PV}}}{\hat{\nu}_{\text{PV}}} \quad (9)$$

where $\hat{\nu}_{\text{PV}}$ denotes the ensemble's standard deviation averaged over the previous month. $\kappa_{\text{PV}}^{\text{VD}}$ is used to yield the calibrated ensemble

$$\bar{p}_{\text{PV}}^m = \bar{p}_{\text{PV}}^{m, \text{uncalib}} + \kappa_{\text{PV}}^{\text{VD}} (\bar{p}_{\text{PV}}^{m, \text{uncalib}} - \hat{p}_{\text{PV}}) \quad (10)$$

with the m -th forecast ensemble member $\bar{p}_{\text{PV}}^{m, \text{uncalib}}$ before calibration.

2) *Load Forecast Ensemble*: To generate a forecast for the household load, a linear regression approach is used. To this end our one-year data set is divided into three parts: the training data set and validation set (making up the first half year), and the test data set (the second half of the year), used to evaluate the performance of the control algorithms.

Our forecast model reads

$$p_{\text{Load},k} = \varphi_k^T \theta + \varepsilon \quad (11)$$

where ε denotes the residuals and the vector φ_k the input features at timestep k . These features are a one-hot encoding for the hour of the weekday, the load exactly one week prior, and the load measurement of the last 96 timesteps prior to the forecast. Equation (11) is used for one-step ahead predictions generating a forecast over the full horizon iteratively.

The weights of the linear regression θ are fitted using historical data. A new forecast is generated every $\Delta t_{\text{FC Update}} = 6$ h. In doing so, the data of the last 89 days prior to the initial time of the forecast is used to perform the training to determine θ .

To obtain a measure of the forecast accuracy, the distribution of the residuals is approximated by a Gaussian distribution with mean 0 and standard deviation ν_{Load} which is obtained from training.

The RMSE is calculated in the validation data set. By comparing it with the mean standard deviation of the residual distribution $\hat{\nu}_{\text{Load}}$, the variance deficit factor of the load

$$\kappa_{\text{Load}}^{\text{VD}} = \frac{\text{RMSE}_{\text{Load}}}{\hat{\nu}_{\text{Load}}} \quad (12)$$

is obtained.

With this, a calibrated load forecast ensemble with M_{Load} members is calculated after every $\Delta t_{\text{FC Update}}$. The recursive expression for the calculation of one member reads

$$\bar{p}_{\text{Load},k+1}^m = \varphi_{k+1}^T \theta + \mathcal{N}(0, \kappa_{\text{Load}}^{\text{VD}} \nu_{\text{Load}}) \quad (13)$$

where the standard deviation of the residual distribution ν_{Load} is determined in the respective training period and multiplied with the calibration factor. As discussed, the feature vector φ_{k+1} includes the immediate history of the timeseries. This history is known up to the initial time point of the forecast. When a forecast ensemble member is generated iteratively, every value $\bar{p}_{\text{Load},k}^m$ is used in the input feature vector $\varphi_{k' > k}$.

III. SOLUTION METHODS

As discussed in Section I-A, several schemes exist to control a system in an uncertain environment, in this section we will present the three different solution approaches.

A. Deterministic MPC

Model predictive control (MPC) is a control paradigm which has drawn copious attention in recent years. It is based on solving an optimal control problem at every sampling timestep and applying the first element of the resulting control trajectory to the controlled system. For further details see textbooks such as [20].

For our system, in problem (6) the mean forecast for the residual generation $\hat{\mathbf{R}}$ is taken for the input trajectory \mathbf{R} . The currently measured residual generation is used as the value for R_0 . Then, the resulting deterministic optimization problem is solved using a dynamic programming approach.

B. Scenario-based MPC

A common strategy to account for uncertain forecasts is to use two-stage stochastic MPC based on scenario forecasts. To that end, at each sampling timestep, the current measurement R^* is taken as the forecast for the current timestep

$$R_0^m = R^* \quad (14)$$

$$R_k^m = \bar{R}_k^m \quad \forall k \in \{1, \dots, N\} \quad (15)$$

resulting in a scenario tree branching into M branches within the first timestep. Each branch consists of one ensemble member $\bar{\mathbf{R}}^m$. To get the optimal control input u_0 , the expected cost is optimized.

$$\begin{aligned} \min_{u_0, x_1} \quad & \mathbb{E}_m J^{\text{Scen}}(x_1, u_0, \mathbf{R}) \\ & = \frac{1}{M} \sum_{m=0}^{M-1} [g_0(u_0, R_0^m) + g_N(x_1, \mathbf{R}^m)] \end{aligned} \quad (16)$$

subject to

$$x_1 = f^x(x_0, u_0)$$

where x_0 denotes the initial state of charge and \mathbf{R} the complete forecast ensemble. Furthermore, $g_N(x_1)$ are the terminal costs that emerge from the deterministic optimization of control given the m -th ensemble member. The costs of each branch of the scenario tree can be determined by solving the m independent optimization problems

$$g_N(x_0, \mathbf{R}) = \min_{\{u_k\}_{k=1}^{N-1}, \{x_k\}_{k=1}^N} \sum_{k=1}^{N-1} g(u_k, R_k) + g_N(x_N) \quad (17)$$

subject to

$$\begin{aligned} x_{k+1} &= f^x(x_k, u_k) & \forall k = 0 \dots N-1 \\ x &\in \mathcal{X} & \forall k = 0 \dots N \\ u_k &\in \mathcal{P}(x_k) & \forall k = 0 \dots N-1 \\ x_1 &= x_{\text{init}} \end{aligned}$$

The optimal control problems (17) can be solved with the same algorithm as the problem in Section III-A. The resulting optimal control input u_0 is applied to the system and the procedure is repeated at the next timestep.

C. Dynamic Programming Algorithm for Stochastic MPC

Principally, the expected residual generation and the control inputs at an arbitrary point in the forecast horizon can depend on their realizations up to that point. Therefore, considering the full forecast tree branching at every timestep can be beneficial. This full tree can be considered using stochastic dynamic programming (SDP): an SDP scheme is set up with two states x and R which denote the state of charge and the residual generation respectively. For further information on stochastic dynamic programming, we refer the reader to [21]. The evolution of the state of charge is governed by (2). The residual generation evolves as

$$R_{k+1} = \rho_k + \sigma_k n \equiv \hat{R}_{k+1} + \tau(R_k - \hat{R}_k) + \sigma_k n \quad (18)$$

with the mean forecast \hat{R}_k as well as the persistency parameter τ and the uncertainty parameters $\{\sigma_k\}_{k=1}^N$. The second term in (18) incorporates the assumption that the current measurement for the residual generation is a good estimate for the close future. The parameter $\tau \in [0, 1]$ determines how fast the weight of current measurement decreases over the horizon. The last term in (18) includes a measure for forecast uncertainty from one timestep to the next. It is modeled as a Gaussian noise n with standard deviation σ_k .

The probabilistic forecast ensemble can be used to determine the possibly time-dependent model parameter σ_k . The method of how a maximum likelihood fit is used to do so, can be found in the appendix. The resulting expression reads

$$\sigma_k = \sqrt{\frac{1}{M} \sum_{m=0}^{M-1} (\bar{R}_{k+1}^m - \rho_{k+1}^m)^2} \quad (19)$$

where $\rho_{k+1}^m = \bar{R}_{k+1}^m + \tau(\rho_k^m - R_k^m)$ is defined recursively. A time independent σ can be obtained by averaging over the time horizon of the forecast.

To use dynamic programming, the state spaces of x and R have to be discretized into n_x and n_R states respectively. The state space discretization into $\mathcal{X}_{\text{Discr}}$ also leads to a discretization of the control space

$$\mathcal{U}(x_k) \equiv \mathcal{P} \cap \{u^i = (f^x)^{-1}(x^i | x_k) \quad \forall x^i \in \mathcal{X}_{\text{Discr}}\} \quad (20)$$

with the system model from \mathcal{P} , \mathcal{X} and $f^x(x_k, u_k)$. Limiting the control variable to this set, asserts the state constraints.

For every timestep and discrete state a "cost-to-go" $J_k(x_k, R_k)$ is computed. To start, terminal costs are allocated for the state at the end of the horizon

$$J_N(x_N, R_N) = g_N(x_N). \quad (21)$$

Then, iterating backwards, the cost-to-go is computed for each point in the horizon

$$J_k(x_k, R_k) = \min_{u_k \in \mathcal{U}(x_k)} g_k(u_k, R_k) + \mathbb{E}_{R_{k+1}} [J_{k+1}(f^x(x_k, u_k), R_{k+1})] \quad (22)$$

This implies the policies

$$\mu(x_k, R_k) = \operatorname{argmin}_{u_k \in \mathcal{U}(x_k)} g_k(u_k, R_k) + \mathbb{E}_{R_{k+1}} [J_{k+1}(f^x(x_k, u_k), R_{k+1})]. \quad (23)$$

mapping a state at timestep k to an optimal control action. The expectation value is computed over the distribution of R_{k+1} given by (18).

These policies are calculated at every update to the external forecast after $\Delta t_{\text{FC Update}} = 6$ h. During operation, the optimal control action u is determined from the respective policy at each sampling timestep using the measured values x^* and R^* .

IV. BENCHMARK CASE STUDY

The goal of this study is to estimate how well different methods mitigate forecast uncertainty. To do so, a simulation is carried out. As a benchmark system we consider a grid connected PV battery system coupled via the AC household bus. The system fulfills all assumptions made in Section II-A. The evolution of the state of charge is governed by the battery power u_k

$$x_{k+1} = f^x(x_k, u_k) := x_k - p_{\text{Eff}}(u_k) \cdot \frac{\Delta t}{C_{\text{Bat}}} \quad (24)$$

where $C_{\text{Bat}} = 5$ kWh is the effective capacity of the battery and

$$p_{\text{Eff}}(u_k) = \begin{cases} (1 - \epsilon)(u_k + p_{\text{Loss}}(u_k)) & \text{if } u_k < 0 \\ (1 + \epsilon)(u_k + p_{\text{Loss}}(u_k)) & \text{if } u_k > 0 \\ 0 & \text{if } u_k = 0 \end{cases} \quad (25)$$

is the effective charging power. The losses stem from the static battery efficiency $\epsilon = \sqrt{0.96}$ and the dynamic inverter losses

$$p_{\text{Loss}}(u_k) = p_{\text{nom}} \left(p_a + u_a \frac{u_k}{p_{\text{nom}}} + r_a \left(\frac{u_k}{p_{\text{nom}}} \right)^2 \right) \quad (26)$$

where we use the typical parameters $p_a = 0.00387$, $u_a = 0.0178$ and $r_a = 0.0272$. For the nominal inverter power we use $p_{\text{nom}} = 2.5$ kW. The operation region of the inverter is given by

$$\mathcal{P} = [-p_{\text{nom}}, -0.05 p_{\text{nom}}] \cup \{0\} \cup [0.05 p_{\text{nom}}, p_{\text{nom}}]. \quad (27)$$

Note that when combining (25) and (27), feasibility is guaranteed as $0 \in \mathcal{U}$ at all times. The state of charge is further limited to the interval $x \in \mathcal{X} = [0, 1]$.

The power of the photovoltaic generator, the household load and the battery is balanced via the public electricity grid. We consider a feed-in limitation into the electric grid of 50% of the PV nominal power. Here we simulate a PV generator

with a nominal power of 5 kW and therefore a feed-in limit of $p_{\text{Lim}} = 2.5 \text{ kW}$. If the residual generation exceeds the feed-in limit, PV power is curtailed. The stage costs are defined as the cost for electricity supplied and a remuneration for electricity fed into the grid

$$g_k(u_k, R_k) = \begin{cases} -c_s(u_k + R_k) & \text{if } u_k + R_k < 0 \\ -c_f(u_k + R_k) & \text{if } 0 < u_k + R_k < p_{\text{Lim}} \\ -c_f p_{\text{Lim}} & \text{else} \end{cases} \quad (28)$$

where $c_s = 28 \text{ ct/kWh}$ and $c_f = 12.3 \text{ ct/kWh}$ are the price for electricity supply and the feed-in tariff respectively. The terminal costs are defined using the average of both cost coefficients

$$g_N(x_N) = -x_N \frac{c_s + c_f}{2}. \quad (29)$$

In the cost structure defined in (28) charging the battery with PV generation leads to cost savings by avoiding supply from the public grid. However, if the battery is charged too early high PV generation can no longer be stored and must be curtailed. The goal of optimal operation is to find the best balance between self-consumption through early charging and postponing charging from PV in order to avoid curtailment losses.

As a forecast for the residual generation we use a procedure as presented in Section II-C. We have $M_{\text{PV}} = M_{\text{Load}} = 50$ ensemble members for the PV and load forecast resulting in 2500 members of the residual generation ensemble.

A. Compared Algorithms

To benchmark these different methods, a simulation is carried out. Four algorithms have been compared.

- **Deterministic MPC (Det. MPC):** No modeling of forecast uncertainty as described in Section III-A.
- **Scenario based MPC (Scen. MPC):** A two-stage MPC approach such as in Section III-B is implemented. Out of the 2500 available scenarios 100 are selected.
- **Multi-stage MPC using fitted σ from ensemble (SDP):** The algorithm described in III-C is used to generate policies using a constant value for σ fitted from the ensemble forecast for each policy generation.
- **Multi-stage MPC using fitted σ_k from ensemble (Time-dep SDP):** The algorithm described in III-C is used to generate policies using values for σ_k which vary over the horizon.

B. Simulation Results

The methods have been compared with respect to their curtailment losses relative to the overall PV production and an electricity bill calculated with the cost function given in (28). Furthermore, the self-sufficiency Σ_{Self} , is defined as the fraction of overall household demand produced by PV.

From the yearlong data, a half year was used to train the load and PV forecast algorithms. The simulations estimating controller performance were executed on the remaining half year. The results for the compared algorithms are summarized in Table I. The resulting electricity bill (which corresponds to

TABLE I
PERFORMANCE OF DIFFERENT METHODS TO MITIGATE FORECAST UNCERTAINTIES. THE SIMULATIONS ARE DONE FOR THE CALIBRATED FORECAST ENSEMBLE (UPPER PART) AND THE UNCALIBRATED ENSEMBLE (LOWER PART). ON AVERAGE, THE CALIBRATION INCREASED THE STANDARD DEVIATION OF THE FORECAST ENSEMBLE BY A FACTOR OF 1.5.

Method	Σ_{Self}	Relative Curtailment	Electricity bill [Eur]
Det. MPC	43.3 %	1.92 %	135.9
Scen. MPC	45.9 %	1.26 %	125.9
SDP	50.9 %	1.82 %	112.5
Time-dep SDP	51.7 %	1.88 %	110.2
Results for uncalibrated forecast ensemble			
Scen. MPC	45.3 %	1.25 %	127.5
SDP	51.5 %	2.00 %	111.4
Time-dep SDP	51.6 %	1.86 %	110.2

the optimization costs), shows that including a model of the forecast uncertainty has led to a better controller performance. For the scenario based approach this increase was mainly due to avoiding curtailment losses. For the SDP approaches the main reason was the increased self-sufficiency. This can be explained by the difference in the modeling of the residual generation. In the scenario-based scheduling, some scenarios predicted large PV generations and therefore curtailment losses, pushing the optimal charging power to a lower value. These trajectories are considered in SDP as well. However, with the forecast model (18) trajectories that drift towards the mean forecast are weighted more, leading to less sensitivity for curtailment losses.

The time-dependent SDP approach performed slightly better than the time-independent approach. This could be due to a better modeling of the varying forecast uncertainty with the varying PV generation due to the course of the sun.

When comparing the performance of the controller given a calibrated and an uncalibrated ensemble, it becomes apparent that the calibration only slightly changes the performance of the controllers. This suggests that the studied controllers are robust against limited errors in the estimation of forecast uncertainties. The calibration factors were approximately 1.5 in our study. If this robustness remains for larger mismatch of the forecasted and actual forecast uncertainty may be investigated in further studies.

V. OUTLOOK

Four different methods of mitigating forecast uncertainty in optimal operation have been simulated. It has been shown, that considering forecast uncertainties can lead to better performance of a controlled system. Furthermore, our results suggest that a more complex model of the forecast uncertainty further increases the performance.

However, a comprehensive study analyzing different application cases for a larger data set must be done in order to yield more reliable results.

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In Section III-C we presented an algorithm to consider forecast uncertainty in optimization. This scheme includes a Markov chain model for a forecast of the residual generation in (18). Here, we will show, how the parameters $\sigma = [\sigma_0, \dots, \sigma_{N-1}]$ of that model can be determined from an ensemble forecast $\bar{\mathbf{R}}$ using a maximum likelihood estimation.

When using (18), the probability for a one-step prediction of R_{k+1} given the measurement R_k at the previous timestep $k > 0$ as well as the parameter σ_k reads

$$p(R_{k+1}|R_k, \sigma_k) = \frac{1}{\sqrt{2\pi\sigma_k^2}} \exp\left(-\frac{(R_{k+1} - \rho_{k+1})^2}{2\sigma_k^2}\right) \quad (30)$$

with

$$\rho_{k+1} = \hat{R}_{k+1} + \tau(R_k - \hat{R}_k) \quad (31)$$

depending on the previous measurement R_k and mean forecast \hat{R}_k .

In terms of the maximum likelihood estimation, the ensemble forecast $\bar{\mathbf{R}}$ can be seen as M independent measurements

$$y^m = \mathbf{R}^m = [\bar{R}_0^m, \dots, \bar{R}_N^m]^T, \quad (32)$$

for the residual generation $\mathbf{R} = [R_0, \dots, R_N]$.

Bayes rule is used to yield the probability of the complete measurement y^m by generalizing (30) to

$$p(y^m|\sigma) \equiv p(\bar{R}_N^m, \bar{R}_{N-1}^m, \dots, \bar{R}_1^m|\bar{R}_0^m, \sigma) \quad (33)$$

$$= \prod_{k=0}^{N-1} p(\bar{R}_{k+1}^m|\bar{R}_k^m, \sigma_k). \quad (34)$$

With this, we can derive the likelihood P of all M measurements y^m from the forecast ensemble given the parameters σ and the initial values $\{\bar{R}_0^m\}_{m=0}^{M-1}$

$$P(\mathbf{y}|\sigma) = \prod_{m=0}^{M-1} p(y^m|\sigma) \quad (35)$$

with $\mathbf{y} = [y^0, \dots, y^{M-1}]$ denoting the M individual measurements. In order to determine the best fit σ^{Opt} this likelihood is maximized

$$\sigma^{\text{Opt}} = \underset{\sigma}{\operatorname{argmax}} P(\mathbf{y}|\sigma). \quad (36)$$

We transform (36) into the minimization of the negative logarithm of the likelihood

$$\sigma^{\text{Opt}} = \underset{\sigma}{\operatorname{argmin}} [-\log P(\mathbf{y}|\sigma)] \quad (37)$$

where

$$\begin{aligned} F &\equiv -\log P(\mathbf{y}|\sigma) \\ &= \left[\frac{M}{2} \sum_{k=0}^{N-1} \ln(2\pi\sigma_k^2) + \sum_{m=0}^{M-1} \sum_{k=0}^{N-1} \frac{(\bar{R}_{k+1}^m - \rho_{k+1}^m)^2}{2\sigma_k^2} \right]. \end{aligned} \quad (38)$$

With this, problem (37) can be solved analytically by deriving F with respect to σ_k yielding

$$0 = \frac{\partial F}{\partial \sigma_k} = \frac{M}{\sigma_k} - \frac{1}{\sigma_k^3} \sum_{m=0}^{M-1} (\bar{R}_{k+1}^m - \rho_{k+1}^m)^2. \quad (39)$$

This in turn results in the analytic independent expressions for the parameters σ in (19)