# Simulation Methods for Stochastic Storage Problems: A Statistical Learning Perspective

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## Storage Problems

- Managing inventory in the presence of risk
- Sequentially decide when to augment/draw-down inventory given a randomly evolving environment
- Stochastic Switching Control
- Natural Gas Storage facility (underground caverns):
  - Maximize revenue: buy low/sell high
  - Widely used by market participants through bespoke tolling/lease agreements

## Microgrid Battery Management:

- Renewable generation facility (solar or wind) leading to stochastic net demand
- Diesel generator for back-up
- Minimize costs: optimize battery operations
- Avoid blackouts/minimize diesel costs

## Output: Feedback Control



Figure: *Left panel:* action to undertake when injecting into a **gas storage** facility as a function of gas price and current inventory: inject, store, withdraw. *Right panel:* action to undertake when **diesel generator** is off, as a function of current residual demand and inventory: OFF, ON (variable level).

### We are interested in efficient ways of generating these maps.

## Storage Problems as Control

- Abstractly: stochastic control of switching-type
- Stochastic factor P<sub>t</sub> (price, demand, etc)
- Inventory variable It
- ▶ Controlled regime  $m_t \in M$ ; switching costs K(m, m')
- Typically [not required]: (P<sub>t</sub>) is exogenous (follows an SDE); (I<sub>t</sub>) is fully endogenous, determined by (m<sub>t</sub>) (ODE)
- Objective and cost include all of  $(P_t, I_t, m_t)$  and subject to inventory constraints  $I_t \in [I_{\min}, I_{\max}]$
- View m<sub>t</sub> as a persistent regime that is part of the system state and drives system dynamics [dependence vanishes if switching costs are zero]
- Discrete-time formulation

## Natural Gas Storage

- Gas price  $P_t$  stochastic process
- Action space:  $\mathcal{M} = \{+1, 0, -1\}$ : inject, store, withdraw
- Leads to control  $c_t(m, I)$  (cavern pressure) and inventory impact  $dI_t = a(c_t)dt$
- Capacity constraint  $I_t \in [0, I_{max}]$
- $\blacktriangleright$  Discrete/ switching control space: pick the best action from  ${\cal M}$
- ▶ Notation:  $m_{t_{k+1}}$  is the regime on  $[t_k, t_{k+1}]$ , determines  $I_{t_{k+1}}$  (previsible)

## Solution Structure

- Controlled inventory:  $\hat{I}_{t_{k+1}} = \hat{I}_{t_k} + a (c_{t_k}(\hat{m}_{t_{k+1}}(t, P, I, \hat{m}_{t_k}))) \Delta t$
- If P<sub>t</sub> is high inject; if low : withdraw.
- Key output is the control **map** from which recursively read-off  $m^*(t, P_t, I_t, m_t)$ .



Figure: Left panel: snapshot of the control map  $\hat{m}(t, P, I)$  at t = 2.7 years. Top right: a given trajectory of commodity price  $(P_t)$  following logarithmic mean reverting dynamics. Lower right: Corresponding trajectories of controlled inventory  $\hat{l}_t$  starting at  $\hat{l}_0 \in \{0, 500, 1000, 2000\}$ . Obtained from the PR-1D solution scheme.

## Stochastic Control Formulation

Value function

$$V(t_k, P, I, m) = \sup_{\mathbf{m}_{t_k}} \mathbb{E}\left[v(t_k, \mathbf{P}_{t_k}, I_{t_k}, \mathbf{m}_{t_k}) \middle| P_{t_k} = P, I_{t_k} = I, m_{t_k} = m\right]$$

Payoff is 
$$v(t_k, \mathbf{P}_{t_k}, I_{t_k}, \mathbf{m}_{t_k}) := \sum_{s=k}^{K-1} e^{-r(t_s-t_k)} [\pi(P_{t_s}, c_{t_k}(m_{t_{s+1}}))\Delta t - K(m_{t_s}, m_{t_{s+1}})] + e^{-r(T-t_k)}W(P_T, I_T)$$

► Continuation value:  $q(t_k, P, I, m) := \mathbb{E}\left[e^{-r\Delta t}V(t_{k+1}, P_{t_{k+1}}, I, m) \middle| P_{t_k} = P\right]$ .

Dynamic Programming equation

 $V(t_k, P_{t_k}, I_{t_k}, m_{t_k}) = \max_{m \in \mathcal{J}} \mathbb{E} \left[ \pi^{\Delta}(P_{t_k}, m_{t_k}, m) + e^{-r\Delta t} V(t_{k+1}, P_{t_{k+1}}, I_{t_{k+1}}(m), m) \middle| P_{t_k} \right]$ 

• Optimal control  $m_{t_{k+1}}^*(t_k, P_{t_k}, I_{t_k}, m_{t_k})$  is the argmax above.

## Existing Solution Methods

- PDE-based (Chen and Forsyth '08, Thompson '16) degenerate in *I*-coordinate; limited to 1D factor models.
- Regression Monte Carlo: Carmona-L ('10), Denault et al ('13), Boogert and de Jong ('08, '11), Warin ('10), Bauerle and Riess ('16), Malyscheff and Trafalis ('17), Balata and Palczewski ('17),....
- Classic RMC: generate forward paths, use the resulting stochastic mesh to solve the DPE, employ cross-sectional regression for the conditional expectation. Construct pathwise rewards.
- Key challenge for applying RMC is how to handle the endogenous I<sub>t</sub> cannot do global path simulation
  - Inventory path back-propagation and quasi-simulation
  - Treat  $I_t$  as a parameter, solve a collection of 1-D problems in  $P_t$
  - Control randomization

## Regression: The -1D Discretization Trick

- Reduce to a finite number of 1D switching problems by discretizing the inventory *I*, solved in parallel
- $M_l + 1$  levels  $l_0, l_1, \dots, l_{M_l}$ , fit in P for each level, i.e. optimize for  $\hat{h}_j(P) := \vec{\beta}_j^T \vec{\phi}(P)$  for  $j = 0, \dots, M_l$

## Interpolate:

$$\widehat{h}_{t_k}(P,I) := \delta(I) \ \widehat{h}_j(P) + (1 - \delta(I)) \ \widehat{h}_{j+1}(P),$$
where  $\delta(I) = \frac{I - I_j}{I_{j+1} - I_j}.$ 

- Makes the policy smooth in P but not in I; the discretization grid (Im) plays a big role
- Works very well but limited scope



## RMC for Storage: Machine Learning Perspective

- Abstract away the conventional RMC particulars
- The storage model is viewed as stochastic simulator(s) that produces noisy pathwise observations conditional on the control
- Learn the continuation or q-value q(t, P, I, m): cost-to-go conditional on next-step regime m; done recursively over t
- Sub-modules [each has multiple viable schemes]:



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- ▶ Put another way: build an *empirical* approximation to the value function  $V(t, \cdot)$  machine learning

# L. -Maheshwari (2018)

- Develop a template for a simulation-based approach to stochastic storage
- Extend latest Regression Monte Carlo techniques to switching control
- A plug-and-play modular algorithm interpreted as a (machine/statistical) learning problem
- Nests existing literature + offers MANY more choices
- Illustrate with some examples (not meant to benchmark yet): Gas Storage/Microgrid Control
- Contributes to the StOpt library developed by Xavier Warin...

## RMC Background: Optimal Stopping

- State process X, payoff  $h(X_t)$ , discrete-time: t = 1, 2, ..., T
- Objective: maximize reward  $V(t, x) = \sup_{\tau} \mathbb{E}_{t,x} [h(X_{\tau})]$
- ► Solution:  $\tau^* = \inf\{t : X_t \in \mathfrak{S}_t\} \land T$ . Stopping region:  $\mathfrak{S}_t = \{x : V(t, x) = h(x)\}$
- Timing value (aka q-value):

$$T(t,x) := \mathbb{E}_{t,x} \left[ V(t+1, X_{t+1}) \right] - h(x) = \mathbb{E}_{t,x} \left[ h(X_{\tau_{t+1}}) \right] - h(x).$$

- ▶ Then  $\mathfrak{S}_t = \{x : \mathbf{T}(\mathbf{t}, \mathbf{x}) < \mathbf{0}\}$  and  $V(t, x) = h(x) + \max(T(t, x), \mathbf{0})$
- Simplest control problem: compare 2 alternatives and choose the best action
- (Later come back to multiple alternatives and multiple state variables)

## Regression Monte Carlo

- The key step is to compute the conditional expectation
- Recast it as a learning task: put in  $X_t = x$ , get back  $V(t+1, X_{t+1}^{t,x}) = y$
- Want to learn the input/output relationship between x's and y's
- Build an emulator (statistical surrogate) using some training data
- Use the emulator to predict for new test data
- Ingredients:
  - The emulator architecture
  - Training data
  - How to obtain y's in the context of DP
  - Performance metrics

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These questions are well-addressed within the Statistical Learning paradigm

## First-Generation RMC

- Late '90s: Carriere '96, Tsitsiklis-van Roy '00, Longstaff-Schwartz '01
- Emulator architecture: classical OLS regression/linear model
  - Parametrize the emulator via basis functions
  - Empirically estimate the coefficients  $\vec{\alpha}$
- Training data:
  - $x_t^n := X_t^{0,x_0,(n)}$  database of N global  $X_t$ -paths
  - Probabilistic simulation design reflects the distribution of X<sub>t</sub><sup>0,x0</sup>
- Simulator responses:
  - ► TvR:  $y_t^n = \hat{V}(t+1, X_{t+1}^{(n)})$ , one-step look-ahead ► LS:  $\tau' = \inf\{s > t : X_s^{(n)} \in \hat{\mathfrak{S}}_s\}$  and  $y_t^n := h(X_{\tau'}^{(n)})$  – pathwise reward

• Performance metric:  $\sum_{t} \|\hat{V}(t, \cdot) - V(t, \cdot)\|_2$ 

# Longstaff-Schwartz 1.0: $\{x_t, y_t\}^{1:N}$ pairs



- 1-D Bermudan Put in GBM model, K = 40 strike
- Piecewise linear approximation of T(t,x) (10 knots in x) at t = 0.6
- ▶ 50,000  $x_t^n \sim LogNormal$
- wild response distribution + low signal-to-noise
- inefficient design: out-of-the-money
   x<sub>t</sub> > 40 samples are useless
- Non-adaptive regression w/22 degrees of freedom

## Enhancements: RMC v1.5

- Improved regression: adaptive bases; regularized; nonparametric;
- Improved performance metrics/ convergence proofs to handle dependent regressions
- ▶ Belomestny:  $|V(0,x) \hat{V}(0,x)| \leq \mathbb{E}_{0,x} \left[ \sum_{s=0}^{T} |T(s,X_s)| \mathbb{1}_{\{X_s \in Err_s\}} \right]$  where  $Err_t := \mathfrak{S}_t \triangle \hat{\mathfrak{S}}_t = \{x : \text{sign } T(t,x) \neq \text{sign } \hat{T}(t,x)\}.$
- Hybrid methods for high-dimensions: regression + interpolation, regression + PDE
- Take expectations then project vs. Project then take expectations ("Regress Later")
- Warin, Gobet, Oosterlee, Belomestny, Stentoft, Kohler, Bender, Egloff, Tompaidis, ... (4000+ citations to LS)

## Our team in the past 5 years: RMC 2.0

- Templated algorithm with a unified stochastic simulation view. Multiple strategies to be combined in a plug-and-play fashion
- + Adaptive Experimental designs
- + Modern emulator frameworks  $\rightarrow$  Gaussian Process regression
- + Objective is to learn the sign of T(t,x) (rank reward vs continuation) contour-finding
- Multiple links to machine learning (Stats/CS/OR which all have their own terminology)

## Illustrating RMC 2.0: 2D Max Call

- Color-coded according to T(t, x)
- Red contour indicates the stopping boundary
- preferentially target regions where T(t, ·) changes signs
- Use active learning heuristics add x sites where  $\hat{T}(t, x) \simeq 0$  or where  $Sd(\hat{T}(t, x))$  is large
- Bespoke regression + bespoke mesh (100 adaptive sites × 40 replications)



## Dynamic Emulation for Stochastic Storage Problems

- Recall the building blocks of RMC:
- Regression how to approximate the conditional expectation (parametric, non-parametric, bivariate)
- Design which data to use for the regression/experiment design: judiciously selecting simulations to run
- Simulation how to simulate pathwise continuation values
- Combine above with a modular framework that brings mix-and-match capabilities
- Advantages of DAE
  - New choices: nonparametric regression
  - New adaptive designs (rather than one ad hoc proposal)
  - New batched designs
  - Straightforward to modify for different contexts/higher dimensions
  - Easy to incorporate additional bells-and-whistles
- Unifies Optimal Stopping RMC and Storage RMC (single software library)

## Dynamic Emulation Algorithm

**Data:** K (time steps),  $(N_k)$  (simulation budgets per step) // N k and D k can change Generate design  $\mathcal{D}_{K-1,m} := (\mathbf{P}_{K-1}^{\mathcal{D}_{K-1,m}}, \mathbf{I}_{K}^{\mathcal{D}_{K-1,m}})$  of size  $N_{K-1}$  for each  $m \in \mathcal{J}$ . line to line Generate one-step paths  $P_{K-1}^{n,\mathcal{D}_{K-1,m}} \mapsto P_{K}^{n,\mathcal{D}_{K-1,m}}$  for  $n = 1, \ldots, N_{K-1}$  and  $m \in \mathcal{J}$ Terminal condition:  $v_{K,m}^n \leftarrow W(P_K^{n,\mathcal{D}_{K-1,m}}, I_K^{n,\mathcal{D}_{K-1,m}})$  for  $n = 1, \ldots, N_{K-1}, m \in \mathcal{J}$ for  $k = K - 1, \dots, 1$  do // Loop in time-steps for  $m \in \mathcal{J}$  do  $\hat{q}(k,\cdot,\cdot,m) \leftarrow \arg\min_{h_k \in \mathcal{H}_k} \sum_{n=1}^{N_k} |h_k(P_k^{n,\mathcal{D}_{k,m}}, J_{k+1}^{n,\mathcal{D}_{k,m}}) - v_{k+1,m}^n|^2 / \text{Regression}$ Generate design  $\mathcal{D}_{k-1,m} := (\mathbf{P}_{k-1}^{\mathcal{D}_{k-1,m}}, \mathbf{I}_{k}^{\mathcal{D}_{k-1,m}})$  of size  $N_{k-1}$  for each  $m \in \mathcal{J}$ Generate one-step paths  $P_{k-1}^{n,\mathcal{D}_{k-1,m}} \mapsto P_k^{n,\mathcal{D}_{k-1,m}}$  for  $n = 1, \ldots, N_{k-1}$  // TvR style end for  $n = 1, ..., N_{k-1}$  and  $m \in \mathcal{J}$  do // Predict  $m' \leftarrow \operatorname{argmax}_{j \in \mathcal{J}} \{ \pi^{\Delta}(\mathcal{P}_{k}^{n,\mathcal{D}_{k-1,m}},m,j) + \hat{q}(k,\mathcal{P}_{k}^{n,\mathcal{D}_{k-1,m}},I_{k}^{n,\mathcal{D}_{k-1,m}} + a(c_{k}(j))\Delta t,j) \}$  $v_{k}^{n} \leftarrow \pi^{\Delta}(P_{k}^{n,\mathcal{D}_{k-1,m}},m,m') + e^{-r\Delta t}\hat{g}(k,P_{k}^{n,\mathcal{D}_{k-1,m}},I_{k}^{n,\mathcal{D}_{k-1,m}} + a(c_{k}(m'))\Delta t,m')$ end end

return  $\{\hat{q}(k,\cdot,\cdot,m)\}_{k=1,m\in\mathcal{J}}^{K-1}$  // Output is a collection of fitted emulators

## New Regression Proposal: Gaussian Processes

Random field representation of the unknown *q*-value – non-parametric, similar to kernel regression. x ≡ (P, I)

► Squared-Exp. Kernel: 
$$H_{ij} := \kappa(x^i, x^j) = \sigma_f^2 \exp\left(-\frac{1}{2}(x^i - x^j)^T \Sigma^{-1}(x^i - x^j)\right)$$

- ► Hyperparameters: lengthscales  $\Sigma_{ii}$  smoothness in the *i*-th dimension; process variance  $\sigma_f$  controls amplitude, prior mean  $m(\cdot)$ .
- The estimator is in terms of posterior mean/posterior variance, obtained from MVN conditional formulas
- Prediction at x<sub>\*</sub> after training at x:

$$\hat{q}(k, x_*, m) = m(x_*) + H_* \mathbf{H}^{-1}(\mathbf{v}_{\mathbf{k}+1, \mathbf{m}} - m(\mathbf{x}))$$

Fitting a GPR means estimating the hyperparameters

#### Switching Costs Microgrids

# Using GP emulators in DEA

- GPR is good for non-uniform designs since intrinsically a local interpolator; this is crucial for smooth bivariate fits
- GPR has N' degrees of freedom for N' unique  $x_t^n$ 's
- Utilize a batched design (like a MC forest) multiple y's at each x
- Batching improves signal-to-noise ratio and reduces GP regression overhead.
- Posterior variance can be used to create fully adaptive designs ("Active Learning")



#### Switching Costs Microgrids

## Other Regression Choices

- Global Polynomial regression
- Regress only in P; discretize + interpolate in I
- LOESS regression
- Any approximation architecture can be used just need train and predict methods
- ▶ The performance is necessarily linked to the choice of the training data

How to train your DEA:  $\mathcal{D}_k := (x, y)^{1:N_k}$ 

- ▶ In what dimension: Joint -2D (P, I) or -1D by discretize+interpolate in I
- Space-filling vs Targeted explore the entire state space or focus on most relevant regions
- How to generate  $D_k$ : is x randomized or deterministic across runs?
- Replication/Batching re-use same x for multiple simulations, then pre-average pathwise value a la nested MC
- Design Size  $N_k$  can be time-dependent
- Mix-and-match across time-steps

## Comparing Implementations of DEA: Gas Storage

	Regression	Simulation Budget		
Design	Scheme	Low	Medium	Large
Conventional	PR-1D	4,965	5,097	5,231
	GP-1D	4,968	5,107	5,247
	PR-2D	4,869	4,888	4,891
	LOESS-2D	4,910	4,969	5,011
	GP-2D	4,652	5,161	5,243
Space-filling	PR-1D	4,768	4,889	5,028
	GP-1D	4,854	5,064	5,224
	PR-2D	4,762	4,789	4,792
	LOESS-2D	4,747	4,912	4,934
	GP-2D	4,976	5,080	5,133
Adaptive 1D	PR-1D	5,061	5,187	5,246
	GP-1D	5,079	5,195	5,245
Dynamic	GP-1D	5,132	5,225	5,266
	Mixed	5,137	5,205	5,228
Mixture 2D	PR-2D	4,820	4,835	4,834
	LOESS-2D	4,960	4,987	5,003
	GP-2D	5,137	5,210	5,233

Table: Valuation  $\hat{V}(0, 6, 1000)$  (in thousands) using different design-regression pairs and three simulation budgets: Low  $N \simeq 10K$ , Medium  $N \simeq 40K$ , Large  $N \simeq 100K$ .

## Explaining Design Choices

- Probabilistic reflects the distribution of  $(P_t, \hat{l}_t)$
- Space Filling: explore continuation values throughout the input domain. Sub-choices:
  - Quasi Monte Carlo sequences (Sobol)
  - Latin Hypercube Sampling
  - Gridded

Adaptive – target efficient learning of the action boundaries



Figure: Different simulation designs D; in all cases N = 500.

## Some Conclusions

- Space-filling designs do not target enough (unless really fine-tune the input domain)
- Probabilistic designs do not explore enough
- Mixtures of the two work very well
- In 1+1 dimensions, the -1D methods work extremely well, but GP-based -2D regression is competitive
- ▶ The latter requires batched designs for efficient computation
- GPR straightforwardly generalizes to higher dim (cf. 3D example with 2 storage facilities in the paper)

## Add Switching Costs

With switching costs K(m, m') the current regime  $m_t$  becomes part of the state due to preference for inertia. Now have to compute 3 different continuation functions  $\hat{q}(\cdot, m)$ .



Figure: The control maps  $\hat{m}(t, P, I, m)$  at t = 2.7 years for the model with switching costs K(-1, 1) = K(0, 1) = 15000; K(1, -1) = K(0, -1) = 5000; K(1, 0) = K(-1, 0) = 0. The colors are  $\hat{m}_{t+\Delta t} = +1$  (inject, light yellow),  $\hat{m}_{t+\Delta t} = 0$  (store, medium cyan),  $\hat{m}_{t+\Delta t} = -1$  (withdraw, dark blue). The solution used GP-2D regression with Mixture design.

## Microgrids: Avoiding Blackouts

- Renewable generation facility (solar or wind)
- Microgrid demand Net demand X<sub>t</sub> (e.g. follows an OU)
- Battery to smooth out local fluctuations; +diesel generator for back-up

$$\blacktriangleright \text{ Battery } I_{t_{k+1}} = I_{t_k} + a(c_{t_k})\Delta t = I_{t_k} + B_{t_k}\Delta t$$

• Diesel is OFF or ON 
$$(m = 1)$$
 with output  
 $c_{t_k}(1) = X_{t_k} \mathbf{1}_{\{X_{t_k} > 0\}} + B_{\max} \wedge \frac{I_{\max} - I_{t_k}}{\Delta t}$ 

► Battery output for balancing purposes:  

$$B_{t_k} := a(c_{t_k}) = -\frac{I_{t_k}}{\Delta t} \lor (B_{\min} \lor (c_{t_k} - X_{t_k}) \land B_{\max}) \land \frac{I_{\max} - I_{k_k}}{\Delta t}$$

► Imbalance  $S_{t_k} = c_{t_k} - X_{t_k} - B_{t_k}$  – should be zero

• 
$$S_{t_k} > 0$$
 – curtailment;  $S_{t_k} < 0$  – blackout

• Cost: 
$$\pi(c, X) := -c^{\gamma} - |S| \Big[ C_2 \mathbf{1}_{\{S < 0\}} + C_1 \mathbf{1}_{\{S > 0\}} \Big]$$



## Controlling the Diesel



Figure: Left panel: trajectory of the residual-demand  $(X_t)$ , corresponding to policy  $(c_t)$  and the resultant inventory trajectory  $(\hat{l}_t)$ . Middle and right panels: the control policy  $\hat{c}(t, X, I, m)$  at t = 24 hours. Recall that c(0) = 0 whenever the diesel is OFF. All panels are based on GP-2D regression and Mixture design  $\mathcal{D} = \mathcal{P}_2(0.5N) \cup \mathcal{L}_2(0.5N)$ .

## DEA for Microgrid Control

Straightforward adaptation; Discretize potential diesel output,  $m \in \{0, 1, 2, ..., 10\}$ 



- Joint regression together with a mixture design wins again
- Discretization in I works less well because the solution is more nonlinear
- Quite different setup, but results are consistent with the storage example

## Looking Ahead: RMC v3.0

- RMC is poised to be a centerpiece of Applied Stochastics
- Export the outlined ideas to:
  - Quantitative Finance: XVA, parametric pricing/hedging
  - Risk Management: (T)VaR estimation, capital requirements
  - Probability: BSDEs
  - Control: approximate dynamic programming
  - OR/UQ: stochastic simulation
- Ultimate goals: speed; scalability; efficiency; adaptivity
- ▶ Handle more complicated (i) optimization in *m*; (ii) risk attitudes; (iii) constraints

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Thank You!