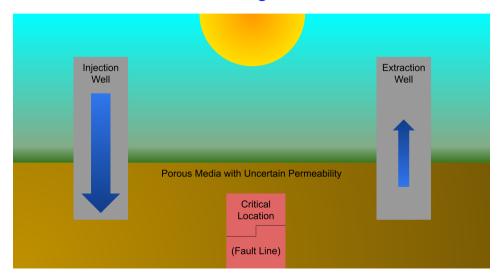
Probabilistic Models for PDEs with Random Coefficients

Aleksei G. Sorokin 1,2 Aleksandra Pachalieva 1 Dan O'Malley 1 Mac Hyman 1 Fred J. Hickernell 2 Nick Hengartner 1

 1 Los Alamos National Laboratory. 2 Illinois Institute of Technology, Department of Applied Mathematics. LA-UR 23-28111

Control Extraction Rate to Manage Pressure at Critical Location

Control Extraction Rate to Manage Pressure at Critical Location



Random Permiability in Porous Media Induces Random Pressure

¹Aleksandra Pachalieva et al. "Physics-informed machine learning with differentiable programming for heterogeneous underground reservoir pressure management". In: Scientific Reports 12.1 (2022), p. 18734.

Random Permiability in Porous Media Induces Random Pressure

Darcy's equation $\nabla \cdot (G(x) \cdot \nabla p(E,G,x)) = f(E,x)$ models pressure in porous media

- G(x) a **random** Gaussian permeability field, known only by statistical properties
- p(x) the **random** pressure solution

¹Aleksandra Pachalieva et al. "Physics-informed machine learning with differentiable programming for heterogeneous underground reservoir pressure management". In: Scientific Reports 12.1 (2022), p. 18734.

Random Permiability in Porous Media Induces Random Pressure

Darcy's equation $\nabla \cdot (G(x) \cdot \nabla p(E,G,x)) = f(E,x)$ models pressure in porous media

- G(x) a random Gaussian permeability field, known only by statistical properties
- p(x) the **random** pressure solution

Following Pachalieva et al.¹, we model the *flow rate* as

$$f(x,E) = \begin{cases} I, & x = x_{\text{injection}} \\ -E, & x = x_{\text{extraction}} \\ 0, & \text{else} \end{cases}$$

- *I*, the **fixed** *injection rate*
- E, the variable extraction rate

¹Aleksandra Pachalieva et al. "Physics-informed machine learning with differentiable programming for heterogeneous underground reservoir pressure management". In: Scientific Reports 12.1 (2022), p. 18734.

Choose Extraction Rate ${\cal E}$ to Rarely Overpressurizes a Critical Location

Choose Extraction Rate ${\cal E}$ to Rarely Overpressurizes a Critical Location

- Given critical location x_{critical} e.g. fault line
- ullet Given pressure threshold $ar{p}$ at the critical location
- $p^c(E,G) := p(E,G,x_{critical})$, the *critical pressure*

Want **online** choice of smallest E which gives high *confidence*

$$P(p^c(E,G) \le \bar{p})$$

in keeping low enough pressure at the critical location

Birds-Eye View



Choose Extraction Rate ${\cal E}$ to Rarely Overpressurizes a Critical Location

- Given critical location x_{critical} e.g. fault line
- ullet Given pressure threshold $ar{p}$ at the critical location
- $p^c(E,G) := p(E,G,x_{critical})$, the *critical pressure*

Want **online** choice of smallest E which gives high $\emph{confidence}$

$$P(p^c(E,G) \le \bar{p})$$

in keeping low enough pressure at the critical location

Injection Well Extraction Well

Critical Location

Birds-Eve View

Challenges

- Must approximate $P(p^c(E,G) \leq \bar{p})$ for many different E values
- Approximating $P(p^c(E,G) \leq \bar{p})$ requires many samples of G(x) e.g. over 10,000

Represent G(x) as an Infinite Sum, Approximate G(x) by a Finite Sum

Represent G(x) as an Infinite Sum, Approximate G(x) by a Finite Sum

Karhunen-Loève series expansion of permeability field G(x)

$$G(x) = \sum_{j=1}^{\infty} \sqrt{\lambda_j} Z_j \varphi_j(x)$$

$$Z_1, Z_2, \dots \stackrel{\mathsf{IID}}{\sim} \mathcal{N}(0, 1)$$

Represent G(x) as an Infinite Sum, Approximate G(x) by a Finite Sum

Karhunen-Loève series expansion of permeability field G(x)

$$G(x) = \sum_{j=1}^{\infty} \sqrt{\lambda_j} Z_j \varphi_j(x)$$

$$Z_1, Z_2, \dots \stackrel{\mathsf{IID}}{\sim} \mathcal{N}(0, 1)$$

Since $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \ldots$, we approximate G(x) by a sum of s terms

$$G(x) \approx \sum_{j=1}^{s} \sqrt{\lambda_j} Z_j \varphi_j(x)$$

$$\mathbf{Z} = (Z_1, \dots, Z_s)^T \sim \mathcal{N}(0, I_s)$$

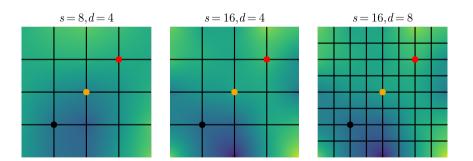
Numerical Solution $p_{s,d}^c(E, \mathbf{Z})$ Approximates True Solution $p^c(E,G)$

s, KL Dimension: $G(x) \approx \sum_{j=1}^s \sqrt{\lambda_j} Z_j \varphi_j(x)$ and $\mathbf{Z} = (Z_1, \dots, Z_s)^T \sim \mathcal{N}(0, I_s)$

d, **Discretization Dimension**: Mesh width 1/d in each physical dimension

Numerical Solution $p_{s,d}^c(E, \mathbf{Z})$ Approximates True Solution $p^c(E,G)$

- s, KL Dimension: $G(x) \approx \sum_{i=1}^{s} \sqrt{\lambda_i} Z_i \varphi_i(x)$ and $\mathbf{Z} = (Z_1, \dots, Z_s)^T \sim \mathcal{N}(0, I_s)$
- d, Discretization Dimension: Mesh width 1/d in each physical dimension



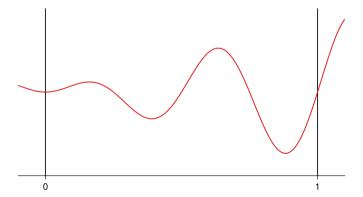
Numerical solution uses DPFEHM: https://github.com/OrchardLANL/DPFEHM.jl

Assume
$$p_{s,d}^c = p^c + \varepsilon$$
, $\varepsilon \sim \mathcal{N}(0, \zeta_{s,d})$

numerical solution = solution + Gaussian noise

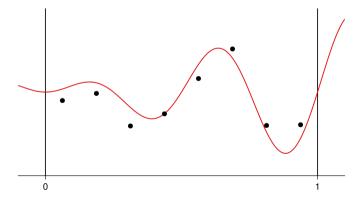
Assume
$$p_{s,d}^c = p^c + \varepsilon$$
, $\varepsilon \sim \mathcal{N}(0, \zeta_{s,d})$

numerical solution = solution + Gaussian noise



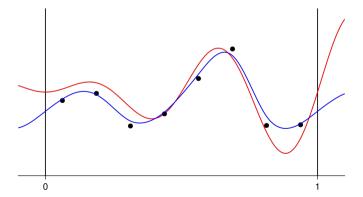
Assume
$$p_{s,d}^c = p^c + \varepsilon$$
, $\varepsilon \sim \mathcal{N}(0, \zeta_{s,d})$

numerical solution = solution + Gaussian noise



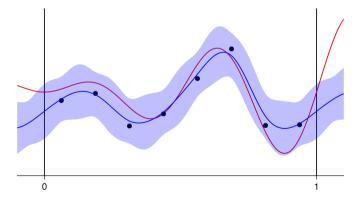
Assume
$$p_{s,d}^c = p^c + \varepsilon$$
, $\varepsilon \sim \mathcal{N}(0, \zeta_{s,d})$

numerical solution = solution + Gaussian noise



Assume
$$p_{s,d}^c = p^c + \varepsilon$$
, $\varepsilon \sim \mathcal{N}(0, \zeta_{s,d})$

numerical solution = solution + Gaussian noise



²R. Jagadeeswaran and Fred J. Hickernell. "Fast automatic Bayesian cubature using lattice sampling". In: Statistics and Computing 29.6 (2019), pp. 1215–1229. ISSN: 1573-1375. DOI: 10.1007/s11222-019-09895-9. URL: http://dx.doi.org/10.1007/s11222-019-09895-9.

³Rathinavel Jagadeeswaran and Fred J Hickernell. "Fast Automatic Bayesian Cubature Using Sobol Sampling". In: Advances in Modeling and Simulation: Festschrift for Pierre L'Ecuyer. Springer, 2022, pp. 301–318.

• Want GP fit to large number of samples nodes e.g. n > 10,000

²R. Jagadeeswaran and Fred J. Hickernell. "Fast automatic Bayesian cubature using lattice sampling". In: Statistics and Computing 29.6 (2019), pp. 1215–1229. ISSN: 1573-1375. DOI: 10.1007/s11222-019-09895-9. URL: http://dx.doi.org/10.1007/s11222-019-09895-9.

³Rathinavel Jagadeeswaran and Fred J Hickernell. "Fast Automatic Bayesian Cubature Using Sobol Sampling". In: Advances in Modeling and Simulation: Festschrift for Pierre L'Ecuyer. Springer, 2022, pp. 301–318.

- Want GP fit to large number of samples nodes e.g. n > 10,000
- Classic GPs cost $\mathcal{O}(n^3)$ to fit

²R. Jagadeeswaran and Fred J. Hickernell. "Fast automatic Bayesian cubature using lattice sampling". In: Statistics and Computing 29.6 (2019), pp. 1215–1229. ISSN: 1573-1375. DOI: 10.1007/s11222-019-09895-9. URL: http://dx.doi.org/10.1007/s11222-019-09895-9.

³Rathinavel Jagadeeswaran and Fred J Hickernell. "Fast Automatic Bayesian Cubature Using Sobol Sampling". In: Advances in Modeling and Simulation: Festschrift for Pierre L'Ecuyer. Springer, 2022, pp. 301–318.

- Want GP fit to large number of samples nodes e.g. n > 10,000
- Classic GPs cost $\mathcal{O}(n^3)$ to fit
- Quasi-random nodes with matching kernels produces nice kernel matrices

²R. Jagadeeswaran and Fred J. Hickernell. "Fast automatic Bayesian cubature using lattice sampling". In: Statistics and Computing 29.6 (2019), pp. 1215–1229. ISSN: 1573-1375. DOI: 10.1007/s11222-019-09895-9. URL: http://dx.doi.org/10.1007/s11222-019-09895-9.

³Rathinavel Jagadeeswaran and Fred J Hickernell. "Fast Automatic Bayesian Cubature Using Sobol Sampling". In: Advances in Modeling and Simulation: Festschrift for Pierre L'Ecuyer. Springer, 2022, pp. 301–318.

- Want GP fit to large number of samples nodes e.g. n > 10,000
- Classic GPs cost $\mathcal{O}(n^3)$ to fit
- Quasi-random nodes with matching kernels produces nice kernel matrices
 - Lattice sequence nodes + periodic shift invariant kernels \rightarrow circulant matrices²

²R. Jagadeeswaran and Fred J. Hickernell. "Fast automatic Bayesian cubature using lattice sampling". In: Statistics and Computing 29.6 (2019), pp. 1215–1229. ISSN: 1573-1375. DOI: 10.1007/s11222-019-09895-9. URL: http://dx.doi.org/10.1007/s11222-019-09895-9.

³Rathinavel Jagadeeswaran and Fred J Hickernell. "Fast Automatic Bayesian Cubature Using Sobol Sampling". In: Advances in Modeling and Simulation: Festschrift for Pierre L'Ecuyer. Springer, 2022, pp. 301–318.

- Want GP fit to large number of samples nodes e.g. n > 10,000
- Classic GPs cost $\mathcal{O}(n^3)$ to fit
- Quasi-random nodes with matching kernels produces nice kernel matrices
 - ullet Lattice sequence nodes + periodic shift invariant kernels o $\it{circulant}$ matrices 2
 - Digital sequence nodes + digitally shift invariant kernels \rightarrow block Toeplitz matrices³

²R. Jagadeeswaran and Fred J. Hickernell. "Fast automatic Bayesian cubature using lattice sampling". In: Statistics and Computing 29.6 (2019), pp. 1215–1229. ISSN: 1573-1375. DOI: 10.1007/s11222-019-09895-9. URL: http://dx.doi.org/10.1007/s11222-019-09895-9.

³Rathinavel Jagadeeswaran and Fred J Hickernell. "Fast Automatic Bayesian Cubature Using Sobol Sampling". In: Advances in Modeling and Simulation: Festschrift for Pierre L'Ecuyer. Springer, 2022, pp. 301–318.

- Want GP fit to large number of samples nodes e.g. n > 10,000
- Classic GPs cost $\mathcal{O}(n^3)$ to fit
- Quasi-random nodes with matching kernels produces nice kernel matrices
 - \bullet Lattice sequence nodes + periodic shift invariant kernels \rightarrow circulant $\mathsf{matrices}^2$
 - ullet Digital sequence nodes + digitally shift invariant kernels o block Toeplitz matrices 3
- Solving systems with these nice kernel matrices costs $\mathcal{O}(n \log n)$

²R. Jagadeeswaran and Fred J. Hickernell. "Fast automatic Bayesian cubature using lattice sampling". In: Statistics and Computing 29.6 (2019), pp. 1215–1229. ISSN: 1573-1375. DOI: 10.1007/s11222-019-09895-9. URL: http://dx.doi.org/10.1007/s11222-019-09895-9.

³Rathinavel Jagadeeswaran and Fred J Hickernell. "Fast Automatic Bayesian Cubature Using Sobol Sampling". In: Advances in Modeling and Simulation: Festschrift for Pierre L'Ecuyer. Springer, 2022, pp. 301–318.

- Want GP fit to large number of samples nodes e.g. n > 10,000
- Classic GPs cost $\mathcal{O}(n^3)$ to fit
- Quasi-random nodes with matching kernels produces nice kernel matrices
 - Lattice sequence nodes + periodic shift invariant kernels \rightarrow circulant matrices²
 - Digital sequence nodes + digitally shift invariant kernels \rightarrow block Toeplitz matrices³
- Solving systems with these nice kernel matrices costs $\mathcal{O}(n \log n)$
- \therefore Can construct GPs with $\mathcal{O}(n\log n)$ cost when we have control over nodes **Object** details



²R. Jagadeeswaran and Fred J. Hickernell. "Fast automatic Bayesian cubature using lattice sampling". In: Statistics and Computing 29.6 (2019), pp. 1215-1229. ISSN: 1573-1375. DOI: 10.1007/s11222-019-09895-9. URL: http://dx.doi.org/10.1007/s11222-019-09895-9.

³Rathinavel Jagadeeswaran and Fred J Hickernell. "Fast Automatic Bayesian Cubature Using Sobol Sampling". In: Advances in Modeling and Simulation: Festschrift for Pierre L'Ecuver, Springer, 2022, pp. 301-318.

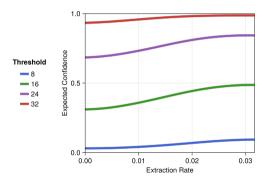
• Approximate upper bound $\bar{\zeta}_{s,d}$ by tracking convergence as fidelity increases • details

- Approximate upper bound $\bar{\zeta}_{s,d}$ by tracking convergence as fidelity increases details
- Decrease $\zeta_{s,d}$ starting at $\bar{\zeta}_{s,d}$ to optimize Gaussian process likelihood

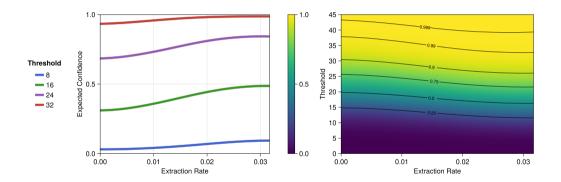
- Approximate upper bound $\zeta_{s,d}$ by tracking convergence as fidelity increases \bullet details
- Decrease $\zeta_{s,d}$ starting at $\overline{\zeta}_{s,d}$ to optimize Gaussian process likelihood
- Hyperparameter optimization also costs $\mathcal{O}(n \log n)$ for specially structured GPs

Estimate $P(p^c(E,G) \leq \bar{p})$ Online with Gaussian Process Surrogate

Estimate $P(p^c(E,G) \leq \bar{p})$ Online with Gaussian Process Surrogate



Estimate $P(p^c(E,G) \leq \bar{p})$ Online with Gaussian Process Surrogate



• **Efficient:** Gaussian process construction in $\mathcal{O}(n \log n)$ instead of $\mathcal{O}(n^3)$ cost

- Efficient: Gaussian process construction in $\mathcal{O}(n \log n)$ instead of $\mathcal{O}(n^3)$ cost
- Error Aware: Gaussian process noise calibrated to numerical error

- **Efficient:** Gaussian process construction in $\mathcal{O}(n \log n)$ instead of $\mathcal{O}(n^3)$ cost
- Error Aware: Gaussian process noise calibrated to numerical error
- Transferable: Methodology applicable to other PDEs with random coefficients

Don't Approximate Confidence $P(p^c(E,G) \leq \bar{p})$ by $P(p^c_{s,d}(E,\mathbf{Z}) \leq \bar{p})$

Don't Approximate Confidence $P(p^c(E,G) \leq \bar{p})$ by $P(p^c_{s,d}(E, \mathbf{Z}) \leq \bar{p})$

• Estimating $P(p^c_{s,d}(E, \mathbf{Z}) \leq \bar{p})$ for many E requires large number of \mathbf{Z} samples

Don't Approximate Confidence $P(p^c(E,G) \leq \bar{p})$ by $P(p^c_{s,d}(E,\boldsymbol{Z}) \leq \bar{p})$

- Estimating $P(p_{s,d}^c(E, \mathbf{Z}) \leq \bar{p})$ for many E requires large number of \mathbf{Z} samples
- \bullet Numerical solutions of $p^c_{s,d}(E,{\pmb Z})$ are too expensive to compute online

Don't Approximate Confidence $P(p^c(E,G) \leq \bar{p})$ by $P(p^c_{s,d}(E,\mathbf{Z}) \leq \bar{p})$

- Estimating $P(p_{s,d}^c(E, \mathbf{Z}) \leq \bar{p})$ for many E requires large number of \mathbf{Z} samples
- \bullet Numerical solutions of $p^c_{s,d}(E,{\bf Z})$ are too expensive to compute online
- $P(p_{s,d}^c(E, \mathbf{Z}) \leq \bar{p}) \neq P(p^c(E,G) \leq \bar{p})$ generally

ullet Can choose sampling nodes $(E_i, {m Z}_i)_{i=1}^n$ to explore the space well

- Can choose sampling nodes $(E_i, \mathbf{Z}_i)_{i=1}^n$ to explore the space well
- ullet Numerical solutions $\{p_{s,d}^c(E_i, \mathbf{Z}_i)\}_{i=1}^n$ can be computed offline

- Can choose sampling nodes $(E_i, \mathbf{Z}_i)_{i=1}^n$ to explore the space well
- Numerical solutions $\{p_{s,d}^c(E_i, \mathbf{Z}_i)\}_{i=1}^n$ can be computed offline
- Surrogate model can be fit offline and evaluated quickly online

- Can choose sampling nodes $(E_i, \mathbf{Z}_i)_{i=1}^n$ to explore the space well
- Numerical solutions $\{p_{s,d}^c(E_i, \mathbf{Z}_i)\}_{i=1}^n$ can be computed offline
- Surrogate model can be fit offline and evaluated quickly online
- ... Inexpensive to estimate confidence $P(p^c(E,G) \leq \bar{p})$ online using surrogate

Assume
$$p_{s,d}^c(t) = p^c(t) + \varepsilon, \qquad \varepsilon \sim \mathcal{N}(0, \zeta_{s,d})$$

numerical solution = solution + Gaussian noise

$$\mbox{Assume } p_{s,d}^c(t) = p^c(t) + \varepsilon, \qquad \varepsilon \sim \mathcal{N}(0,\zeta_{s,d})$$

$$\mbox{numerical solution} = \mbox{solution} + \mbox{Gaussian noise}$$

Gaussian Process Regression

1. Prior mean $\mathbb{E}[p^c(t)]=0$ and covariance $k(t,t'):=\operatorname{Cov}[p^c(t),p^c(t')]=k(t,t').$

$$\text{Assume } p_{s,d}^c(t) = p^c(t) + \varepsilon, \qquad \varepsilon \sim \mathcal{N}(0,\zeta_{s,d})$$

$$\text{numerical solution} = \text{solution} + \text{Gaussian noise}$$

Gaussian Process Regression

- 1. Prior mean $\mathbb{E}[p^c(t)] = 0$ and covariance $k(t,t') := \mathsf{Cov}[p^c(t),p^c(t')] = k(t,t')$.
- 2. Observe $Y = \left(p_{s,d}^c(t_i)\right)_{i=1}^n$

Assume
$$p_{s,d}^c(t)=p^c(t)+\varepsilon, \qquad \varepsilon\sim \mathcal{N}(0,\zeta_{s,d})$$
 numerical solution = solution + Gaussian noise

Gaussian Process Regression

- 1. Prior mean $\mathbb{E}[p^c(t)] = 0$ and covariance $k(t,t') := \mathsf{Cov}[p^c(t),p^c(t')] = k(t,t')$.
- 2. Observe $Y = \left(p_{s,d}^c(t_i)\right)_{i=1}^n$
- 3. Posterior mean $m_n(t) = \mathbb{E}[p^c(t)|Y]$ and covariance $k_n(t,t') = \mathsf{Cov}[p(t),p(t')|Y]$.

$$m_n(t) = K_T(t) \left[K_{TT} + \zeta I_n \right]^{-1} Y$$

costs $\mathcal{O}(n^3)$ where $K_T(t) = (k(t,t_i))_{i=1}^n, K_{TT} = (k(t_i,t_j))_{i,j=1}^n.$

Assume
$$p_{s,d}^c(t)=p^c(t)+\varepsilon, \qquad \varepsilon\sim \mathcal{N}(0,\zeta_{s,d})$$
 numerical solution = solution + Gaussian noise

Gaussian Process Regression

- 1. Prior mean $\mathbb{E}[p^c(t)] = 0$ and covariance $k(t,t') := \mathsf{Cov}[p^c(t),p^c(t')] = k(t,t')$.
- 2. Observe $Y = \left(p_{s,d}^c(t_i)\right)_{i=1}^n$
- 3. Posterior mean $m_n(t) = \mathbb{E}[p^c(t)|Y]$ and covariance $k_n(t,t') = \mathsf{Cov}[p(t),p(t')|Y]$.

$$m_n(t) = K_T(t) \left[K_{TT} + \zeta I_n \right]^{-1} Y$$

costs $\mathcal{O}(n^3)$ where $K_T(t) = (k(t,t_i))_{i=1}^n, K_{TT} = (k(t_i,t_j))_{i,j=1}^n.$

Assume
$$p_{s,d}^c(t)=p^c(t)+\varepsilon, \qquad \varepsilon\sim \mathcal{N}(0,\zeta_{s,d})$$
 numerical solution = solution + Gaussian noise

Gaussian Process Regression

- 1. Prior mean $\mathbb{E}[p^c(t)] = 0$ and covariance $k(t,t') := \mathsf{Cov}[p^c(t),p^c(t')] = k(t,t')$.
- 2. Observe $Y = \left(p_{s,d}^c(t_i)\right)_{i=1}^n$
- 3. Posterior mean $m_n(t) = \mathbb{E}[p^c(t)|Y]$ and covariance $k_n(t,t') = \mathsf{Cov}[p(t),p(t')|Y]$.

$$m_n(t) = K_T(t) \left[K_{TT} + \zeta I_n \right]^{-1} Y$$

costs
$$\mathcal{O}(n^3)$$
 where $K_T(t) = (k(t,t_i))_{i=1}^n, K_{TT} = (k(t_i,t_j))_{i,j=1}^n.$

Quasi-Gaussian Process Regression

Choose special $(t_i)_{i=1}^n$ and k so $[K_{TT} + \zeta I_n]^{-1}Y$ costs $\mathcal{O}(n \log n)$.

Estimating Bound on Standard Deviation of GP Noise

$$\sqrt{\zeta_{s_T,d_T}} = \|p^c - p_{s_T,d_T}^c\| = \sqrt{\mathbb{E}\left[p^c(t) - p_{s_T,d_T}^c(t)\right]^2}, \quad \forall t$$

Rewrite as telescoping sum

$$\sqrt{\zeta_{s_T,d_T}} := \|p^c - p^c_{s_T,d_T}\| \le \sum_{j=T}^{\infty} \|\underbrace{p^c_{s_{j+1},d_j} - p^c_{s_j,d_j}}_{\Delta_{s_{j+1}}}\| + \sum_{j=T}^{\infty} \|\underbrace{p^c_{s_{j+1},d_{j+1}} - p^c_{s_{j+1},d_j}}_{\Delta_{d_{j+1}}}\|.$$

Models $\|\Delta_{s_j}\|=2^{b_s}s_j^{a_s}$ and $\|\Delta_{d_j}\|=2^{b_d}d_j^{a_d}$ with $s_j=v_s2^j$ and $d_j=v_d2^j$ imply

$$\sqrt{\zeta_{s_T,d_T}} \leq \sum_{i=T+1}^{\infty} 2^{b_s} s_j^{a_s} + \sum_{i=T+1}^{\infty} 2^{b_d} d_j^{a_d} = 2^{b_s} v_s^{a_s} \frac{2^{(T+1)a_s}}{1-2^{a_s}} + 2^{b_d} v_d^{a_d} \frac{2^{(T+1)a_d}}{1-2^{a_d}} := \sqrt{\bar{\zeta}_{s_T,d_T}}.$$

Simple Linear Regression Convergence Models

