An adjoint-based optimization method using the solution of gray-box conservation laws

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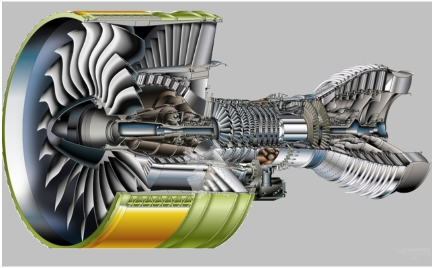
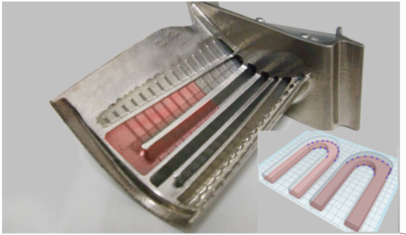
Outline

- Background.
- Estimate gradient by using the space(-time) solution.
- Optimization framework.
- Numerical examples.

Background

- Optimization constrained by conservation law simulation.
- Expensive simulation.
- High dimensional design.
- Code has no adjoint and is proprietary / legacy.





Internal cooling of turbine airfoil
Source: http://www.amaterastvo.biz/eng/technologies.html

Research scope

- Gray-box conservation law simulation:
  - adjoint not available nor implementable.
  - provide space(-time) solution.

	Adjoint	Space(-time) solution	Form of PDE
Black-box	✘	✘	✘
Gray-box	✘	✔	✔
Open-box	✔		

- High-dimensional design space.

Different optimization methods apply

- Black-box: use derivative-free optimization,
  pattern search methods, evolution based methods, etc.
  - not require derivative evaluation.
  - not suitable for high dimensional optimization.
- Open-box: use gradient-based optimization,
  quasi-Newton methods, etc.
  - requires efficient gradient evaluation, generally using adjoint [Lions 71] .
  - suitable for high dimensional optimization.
- Gray-box: treated as black-box. Space(-time) solution wasted!

Problem statement

- Minimize

$$\xi(c) = \int_0^T \int_\Omega j(\boldsymbol{u}, c)\,\mathrm{d}\mathbf{x}\,\mathrm{d}t$$

using a gradient-based optimization method.
$\boldsymbol{u}$: the space-time solution of

$$\dot{\boldsymbol{u}} + \nabla \cdot \boldsymbol{F}(\boldsymbol{u}) = \boldsymbol{q}(\boldsymbol{u}, c)$$

whose $\boldsymbol{F}$ is unknown.

- Steady state solution $\boldsymbol{u}_\infty$

$$\nabla \cdot \boldsymbol{F}(\boldsymbol{u}_\infty) = \boldsymbol{q}(\boldsymbol{u}_\infty, c)$$

is a special case of the time-dependent solution.

Outline

- Background.
- Estimate gradient by using the space(-time) solution.
  - Leverage the space-time solution u.
  - Parameterize the flux.
  - Algorithm for training twin model.
  - Numerical examples.
- Optimization framework.
- Numerical examples.

Estimate adjoint from space-time solution

Away from shock wave, we have

- Primal:

$$\frac{\partial u}{\partial t} + \frac{dF}{du}\frac{\partial u}{\partial x} = q\,, \quad \text{with I.C. and B.C.}$$

- Adjoint:

$$\frac{\partial v}{\partial t} + \frac{dF}{du}\frac{\partial v}{\partial x} = p\,, \quad \text{with I.C. and B.C.}$$

Observations:

- From $u(t,x)$, we get $\frac{\partial u}{\partial t}$, $\frac{\partial u}{\partial x}$.
- From $\frac{\partial u}{\partial t}$, $\frac{\partial u}{\partial x}$, we estimate $\frac{dF}{du}$.
- From $\frac{dF}{du}$, we solve for v.
- Primal / adjoint depend on $\frac{dF}{du}$, not F.

Leverage the space(-time) solution

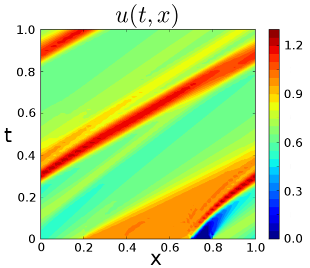
Estimate the gradient:

- Infer the conservation law from the space(-time) solution.
- Estimate the gradient by adjoint method.

Example: infer flux $F(u)$ from space-time solution.

$$\frac{\partial u}{\partial t} + \frac{\partial F(u)}{\partial x} = c(x)$$
$$u(t=0,x) = u_0(x)$$
$$u(t,x=0) = u(t,x=1)$$

Space-time solution

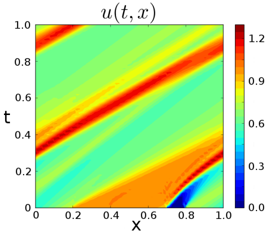


Infer the flux that reproduces the space(-time) solution. The inferred conservation law is called twin model.

Inference can boil down to minimization

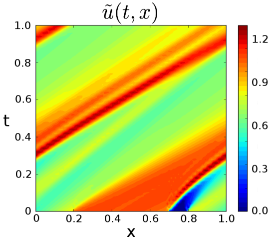
Gray-box model

$$\frac{\partial u}{\partial t} + \frac{\partial F(u)}{\partial x} = c(x)$$
$$u(t=0,x) = u_0(x)$$
$$u(t,x=0) = u(t,x=1)$$



Twin model

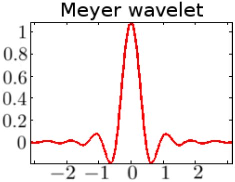
$$\frac{\partial \tilde{u}}{\partial t} + \frac{\partial \tilde{F}(\tilde{u})}{\partial x} = c(x)$$
$$\tilde{u}(t=0,x) = u_0(x)$$
$$\tilde{u}(t,x=0) = \tilde{u}(t,x=1)$$



$$\min_{\tilde{F}} \left\{ \mathcal{M}(\tilde{F},u) \equiv \int_0^1 \int_0^1 (u-\tilde{u})^2_{L_2} \; dt\, dx \right\}$$

Parameterize the flux

- Multi-resolution analysis (MRA) [Mallat 89]
  Wavelet basis
- Adjoint depends on $\nabla_u F$
- Use the integral of wavelet as basis for univariate flux.



$$\phi(u) = \begin{cases} 0 \ , u \to -\infty \\ 1 \ , u \to \infty \end{cases} , \quad \phi(u) = \frac{1}{2}(\tanh(u) + 1)$$

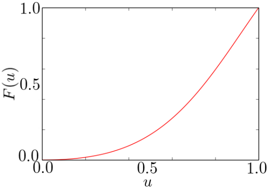
- Univariate flux: use sigmoid function as basis [Mhaskar 92] .

$$\phi_{j,\eta}(u) = \phi(\lambda_j u - \eta) \ , \quad \tilde{F}(u) = \sum_{j,\eta} \alpha_{j,\eta} \phi_{j,\eta}(u)$$

- Multivariate flux: tensor product of univariate sigmoid basis.
- The benefit of sigmoid parameterization will be seen in hindsight.

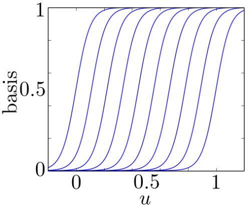
- Consider a Buckley-Leverett equation [Buckley 42]

$$F(u) = \frac{u^2}{1 + 2(1-u)^2}\ , \qquad c : \text{ constant-valued control}$$



- Infer the twin model:

$$\min_{\boldsymbol{\alpha}} \left\{ \underbrace{\int_0^1 \int_0^1 (u - \tilde{u})^2 \; dt\, dx}_{\mathcal{M}} + \lambda \left\|\boldsymbol{\alpha}\right\|_{L_1} \right\}, \quad \lambda > 0$$

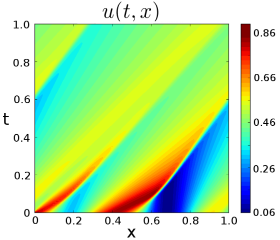


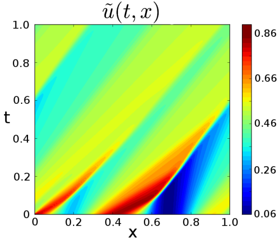
- Estimate $d\xi/dc$ [Kucuk 06]

$$\xi(c) \equiv \int_{x=0}^{1} \big(u(x, t=1; c) - 0.5\big)^2 \,\mathrm{d}x$$

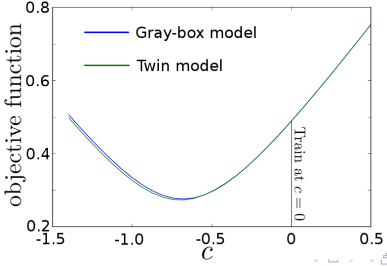
Estimate gradient for BL equation, cont.

- Train a twin model using $u(t, x)$ at $c = 0$.

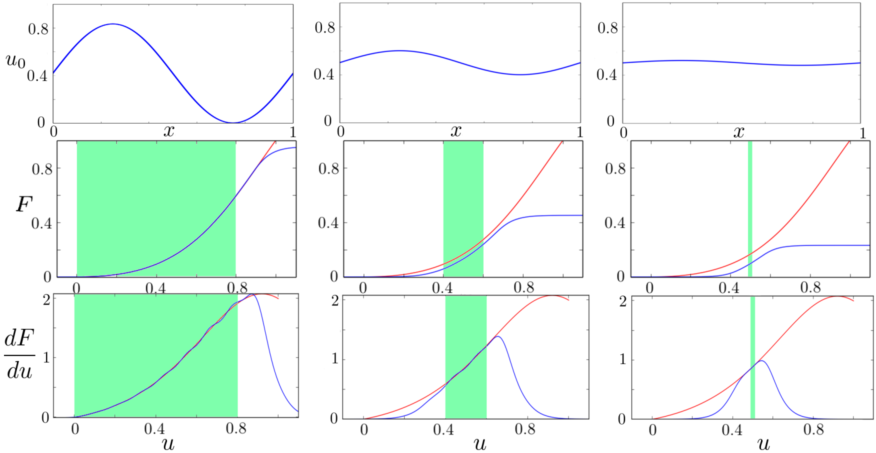




- Twin model can estimate $d\xi/dc$ at $c = 0$.



Only expect match where there is solution



- The range of the discrete gray-box solution $\mathcal{E}_u := [u_{\min}, u_{\max}]$ are green shaded.
- The twin model flux does not affect $\mathcal{M}$ outside the range of the gray-box solution.
- Sigmoid basis can provide local refinement.

Reduce mismatch by adding more basis

Consider improvement of least solution mismatch using more basis functions:

- Basis $[\mathbf{\Phi}_0]$:

$$\mathcal{M}_0^* = \min_{\boldsymbol{\alpha}_0} \mathcal{M}\left(\tilde{F}(\boldsymbol{\alpha}_0), u\right)$$

- Append basis $[\mathbf{\Phi}_0; \mathbf{\Phi}_1]$:

$$\mathcal{M}_{01}^* = \min_{\boldsymbol{\alpha}_0, \boldsymbol{\alpha}_1} \mathcal{M}\left(\tilde{F}(\boldsymbol{\alpha}_0, \boldsymbol{\alpha}_1), u\right)$$

- Mismatch improvement due to appending $\mathbf{\Phi}_1$:

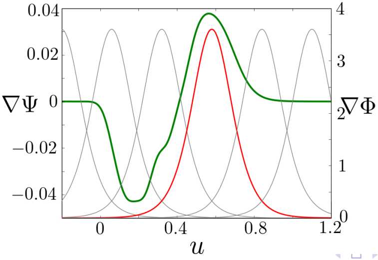
$$\Delta\mathcal{M}^* = \mathcal{M}_0^* - \mathcal{M}_{01}^* \geq 0$$

Rank the basis to be appended

- $$\Delta\mathcal{M}^* \approx -\underbrace{\left(\int_\Omega \frac{\partial\mathcal{M}}{\partial\tilde{F}}\bigg|_{\tilde{F}(\boldsymbol{\alpha}_0^*)} \boldsymbol{\Phi}_1 \,\mathrm{d}u\right)}_{\text{weight vector}} \cdot \boldsymbol{\alpha}_1 = \underbrace{\left(\int_\Omega \nabla\Psi \cdot \nabla\boldsymbol{\Phi}_1 du\right)}_{\text{weight vector}} \cdot \boldsymbol{\alpha}_1 \,,$$

  where $\nabla^2\Psi = \frac{\partial\mathcal{M}}{\partial\tilde{F}}\Big|_{\tilde{F}(\boldsymbol{\alpha}_0^*)}$

- The weight vector ranks the importance of basis. Select the basis with the largest absolute value of weight [Miller 90] .



Represent the sigmoid functions

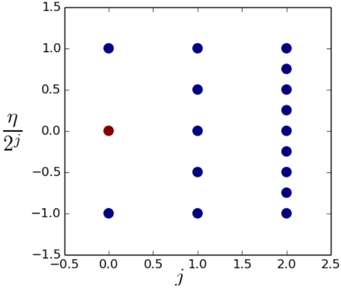
- Consider the sigmoid functions:

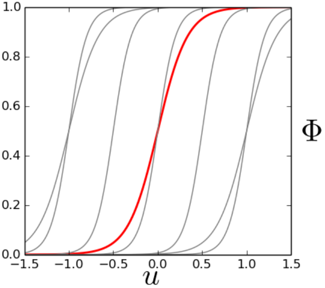
$$\phi_{j,\eta}(u) = \phi(2^j u - \eta)$$

Denote $\phi_{j,\eta}(u)$ by the tuple $\{j, \eta\}$.

$j \in \{j_0, j_0 + 1, j_0 + 2, \cdots\}$ represents resolution. $\frac{\eta}{2^j}$ represents the center of the sigmoid's derivative.

- $j = 0$, $\eta = 0$





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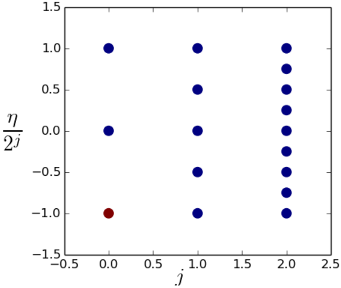
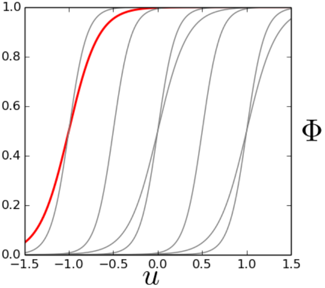
- $j = 0$, $\eta = -1$





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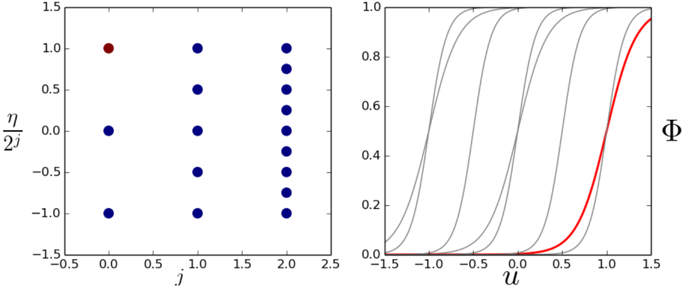
- $j = 0$, $\eta = 1$



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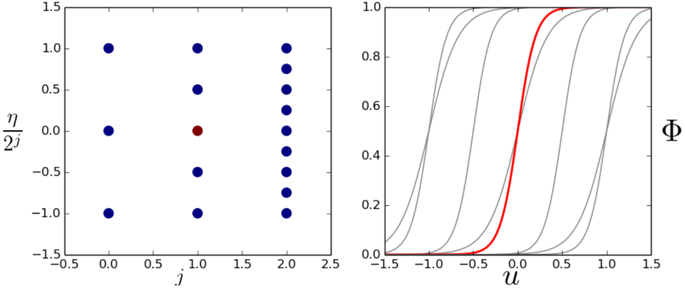
- $j = 1$, $\eta = 0$



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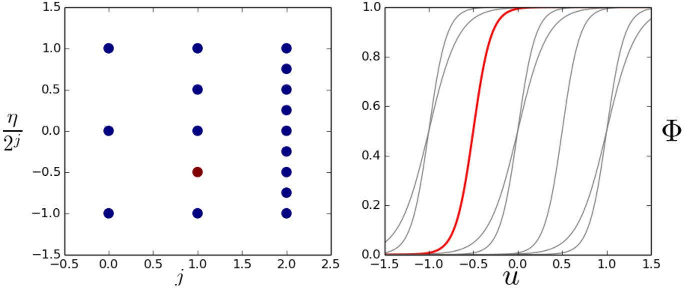

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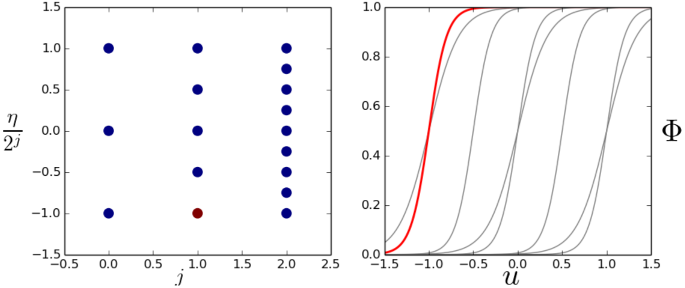
- $j = 1$, $\eta = -2$



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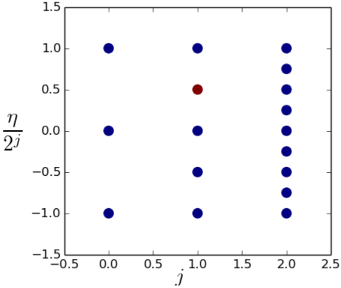
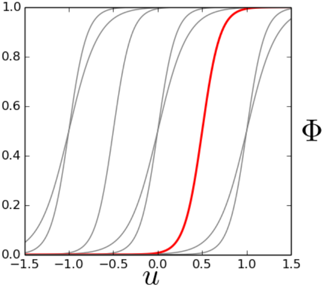
- $j = 1$, $\eta = 1$





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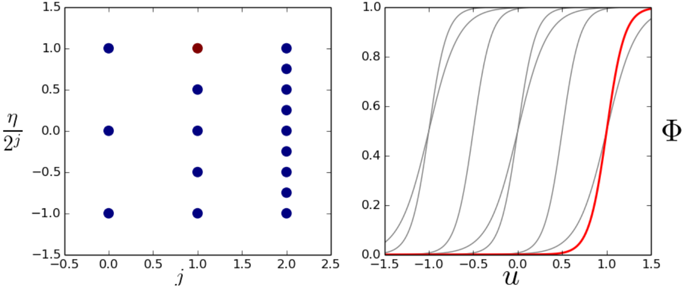
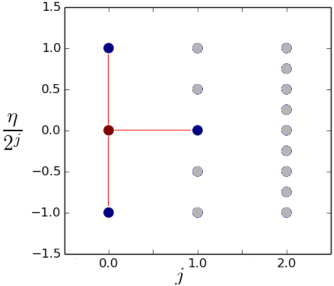
- $j = 1$, $\eta = 2$

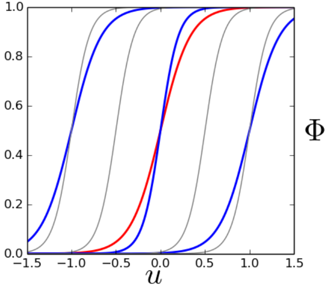


- Define the "neighborhood" of a sigmoid function $\{j, \eta\}$ to be

$$\mathcal{N}(\{j,\eta\}) := \left\{\{j+1, 2\eta\}, \{j, \eta \pm 1\}\right\}$$

- $\mathcal{N}(\{0,0\})$

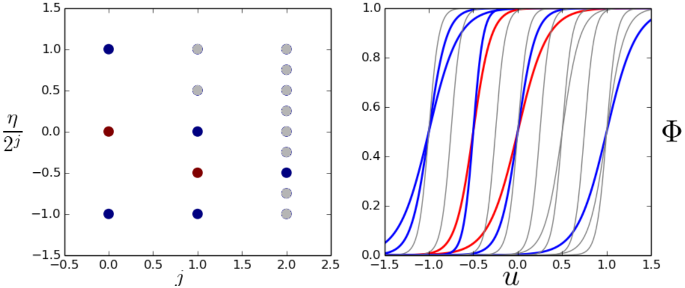




Neighborhood of sigmoid functions

- Define

$$\mathcal{N}(\{j_1,\eta_1\},\cdots,\{j_n,\eta_n\}) := \mathcal{N}(\{j_1,\eta_1\})\bigcup\cdots\bigcup\mathcal{N}(\{j_n,\eta_n\})$$



Select the basis adaptively

- Finite dictionary.
  Can be solved by matching pursuit [Mallat 93]. (forward selection [Friedman 94] , backward prunning [Reed 93]).

  Requires the predetermined basis dictionary contains a subset sufficient for approximation.

- Infinite dictionary. [Jekabsons 10, Blatman 10] .

  Start from an empty or simple dictionary.

  - **Forward step:** (improve accuracy)
    Add a new basis to the dictionary.
  - **Backward step:** (avoid overfit)
    Try to remove a basis from the dictionary.

  Iterate forward / backward steps until the "approximation quality" no longer improves.

Train twin model

Algorithm 1 Train twin model

Input: Basis library $\Psi = \Psi_0$, coefficients $\alpha = \mathbf{0}$. Gray-box solution u

loop

Minimize solution mismatch $\alpha_\Psi \leftarrow \min_\alpha \mathcal{M}\left(\tilde{F}(\Psi, \alpha), u\right)$

if No more basis needed **then**

break

else

Add a basis.

Forward step

if No basis shall be deleted **then**

continue

else

Delete a basis.

Backward step

Output: Ψ, α

Criterion for basis addition / deletion

- Balance approximation accuracy and model complexity. *k*-fold cross validation [Geisser 93] .

- Shuffle u dataset into k disjoint sets: u_1, u_2, $\cdots$, u_k.

  `ravel(`u`);  [`$u_1, \cdots, u_k$`]=shuffle(`u`,k)`

- Train k twin models.

  T_1 = `TrainTwinModel(`$u_2, \cdots, u_k$`)`

  ...

  T_k = `TrainTwinModel(`$u_1, \cdots, u_{k-1}$`)`

- Validate.

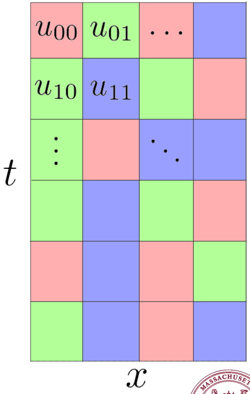
  $\mathcal{M}_1$ = `SolutionMismatch(`T_1`, ` u_1`)`

  ...

  $\mathcal{M}_k$ = `SolutionMismatch(`T_k`, ` u_k`)`

- Compute $\overline{\mathcal{M}}$=`mean(`$\mathcal{M}_1, \cdots, \mathcal{M}_k$`)`

- Add / delete basis if $\overline{\mathcal{M}}$ decreases.



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Output: Ψ, α

Algorithm 1 Train twin model

Input: Basis library $\Psi = \Psi_0$, coefficients $\alpha_\Psi = \mathbf{0}$. $\overline{\mathcal{M}}_0 = \infty$. Gray-box solution u

loop

Minimize solution mismatch $\alpha_\Psi \leftarrow \min_\alpha \mathcal{M}\left(\tilde{F}(\Psi, \alpha), u\right)$

Compute $v = \left.\frac{\partial \mathcal{M}}{\partial \tilde{F}}\right|_{\tilde{F}(\Psi, \alpha_\Psi)}$

Find $\phi_{add} \in \mathcal{N}(\Psi)$ with maximum $\left|\int_\Omega v \phi_{add} \, \mathrm{d}u\right|$

$\Psi \leftarrow \Psi \bigcup \{\phi_{add}\}$, $\alpha \leftarrow \{\alpha, 0\}$

Train twin model via k-fold cross validation, compute $\overline{\mathcal{M}}$

if $\overline{\mathcal{M}} < \overline{\mathcal{M}}_0$ **then**

Accept addition, $\overline{\mathcal{M}}_0 \leftarrow \overline{\mathcal{M}}$, train twin model using all u, update α

else

Reject addition, $\Psi \leftarrow \Psi \backslash \{\phi_{add}\}$, $\alpha \leftarrow \alpha \backslash \{\alpha_{\phi_{add}}\}$, **break**

Compute $v = \left.\frac{\partial \mathcal{M}}{\partial \tilde{F}}\right|_{\tilde{F}(\Psi, \alpha_\Psi)}$

Find $\phi_{del} \in \Psi$ with least $\left|\int_\Omega v \phi_{del} \, \mathrm{d}u\right|$

if $\phi_{del} \neq \phi_{add}$ **then**

$\Psi \leftarrow \Psi \backslash \{\phi_{del}\}$, $\alpha \leftarrow \alpha \backslash \{\alpha_{\phi_{del}}\}$

Train twin model via k-fold cross validation, compute $\overline{\mathcal{M}}$

if $\overline{\mathcal{M}} > \overline{\mathcal{M}}_0$ **then**

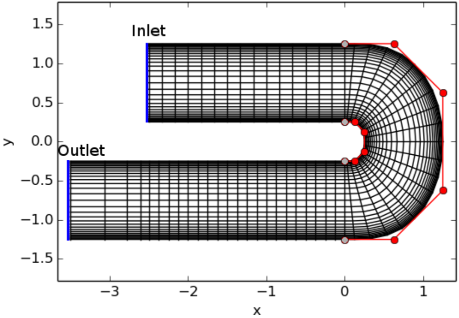
Reject deletion, $\Psi \leftarrow \Psi \bigcup \{\phi_{del}\}$, $\alpha \leftarrow \alpha \bigcup \{\alpha_{\phi_{del}}\}$

else

Accept deletion, train twin model using all u, update α

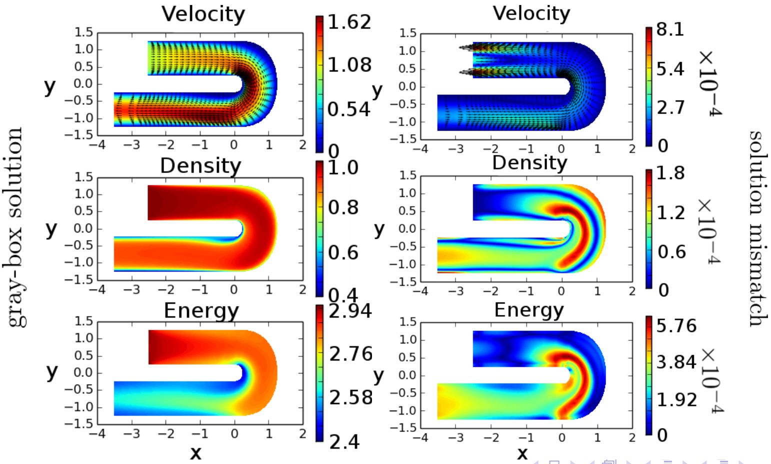
Output: Ψ, α

- Steady-state, 2-D, compressible, laminar Navier-Stokes flow with unknown state equation.
  ($\rho, U \to p$: ideal, van der Waals, Redlich-Kwong [Redlich 49] , etc)
- Geometry

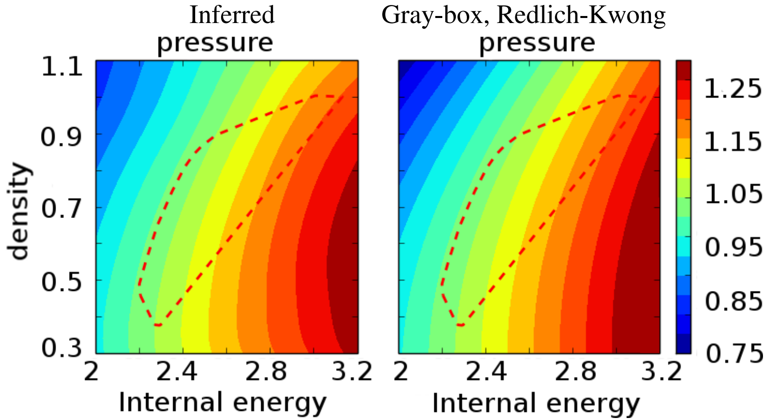


- Bending boundary generated by B-splines.
- Inlet: fixed ρ, p^t. Outlet: fixed p. No slip boundary.

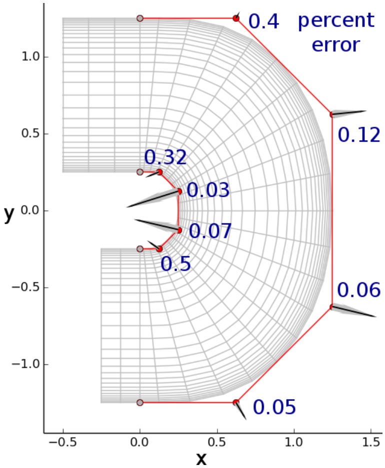
$$\mathcal{M} = w_\rho \int_\Omega |\tilde{\rho}_\infty - \rho_\infty|^2 \, d\mathbf{x} + w_u \int_\Omega |\tilde{u}_\infty - u_\infty|^2 \, d\mathbf{x}$$
$$+ w_v \int_\Omega |\tilde{v}_\infty - v_\infty|^2 \, d\mathbf{x} + w_E \int_\Omega \left|\tilde{E}_\infty - E_\infty\right|^2 \, d\mathbf{x}$$



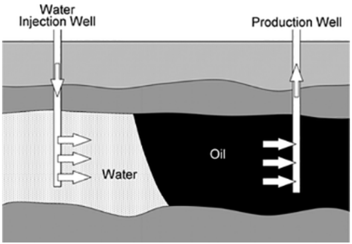
Twin model fits the state equation



- ξ: steady state mass flux rate. c: control points' coordinates.



- Waterflooding for secondary recovery, high water cut.
- Inject polymer to enhance water-phase viscosity and remove residual oil.



Governing equation:

$$\frac{\partial}{\partial t}(\rho_\alpha \phi S_\alpha) + \nabla \cdot (\rho_\alpha \vec{v}_\alpha) = 0\,, \quad \alpha \in \{w, o\}$$
$$\frac{\partial}{\partial t}(\rho_w \phi S_w c) + \nabla \cdot (c\rho \vec{v}_{wp}) = 0$$

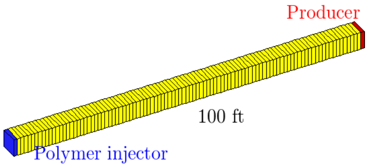
Darcy's law:

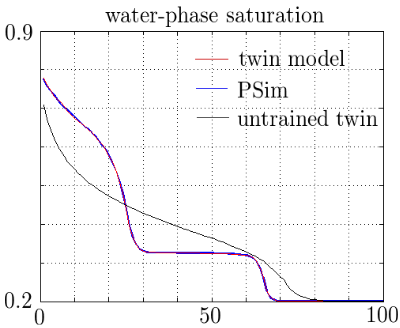
$$\vec{v}_\alpha = -M_\alpha k_{r\alpha} \boldsymbol{K} \cdot (\nabla p - \rho_w g \nabla z), \quad \alpha \in \{w, o\}$$
$$\vec{v}_{wp} = M_{wp} k_{rw} \boldsymbol{K} (\nabla p - \rho_w g \nabla z)$$

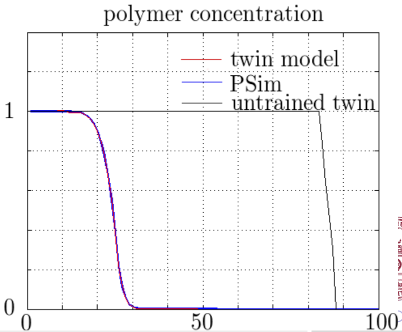
Mobility factors M_o, M_w, M_{wp} depends on S_w, p, c.

Minimize solution mismatch:

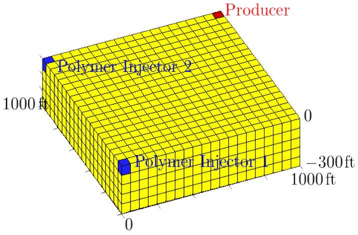
$$\mathcal{M} = w_{S_w} \int_T \int_\Omega |S_w - \tilde{S}_w|^2 d\boldsymbol{x} dt + w_c \int_T \int_\Omega |c - \tilde{c}|^2 d\boldsymbol{x} dt + w_p \int_T \int_\Omega |p - \tilde{p}|^2 d\boldsymbol{x} dt$$

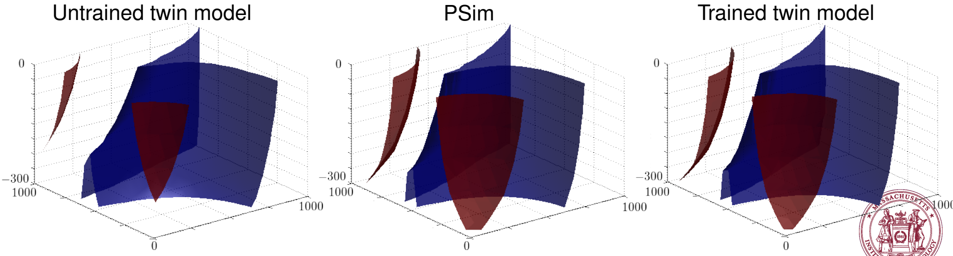






Train the mobility factors, 3D



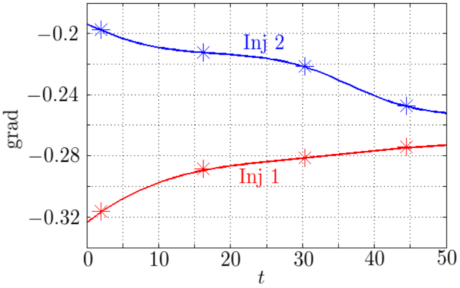


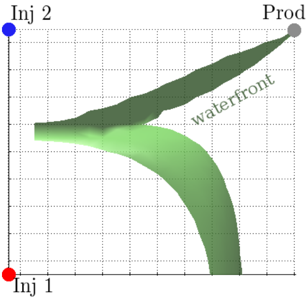
Estimate gradient for injection schedule

Objective: oil residual at $t = 50\,\mathrm{days}$,

$$\xi = \int_{\Omega} \rho_o \phi S_o \,\mathrm{d}\boldsymbol{x}$$

Controls: injection rate schedule at two injectors.





Outline

- Background.
- Estimate gradient by using the space(-time) solution.
- Optimization framework.
  - Model the estimated gradient.
  - Twin-GPO framework.
  - Convergence properties.
  - A numerical example.
- Numerical examples.

Modeling the gradient

- The gradient estimated by twin model is not exactly the true gradient.
  - Gray-box solution under-resolved.
  - Solvers use different numerical implementations.

- To identify the sources of the errors and quantify the errors are difficult. Model the error of each component by "model discrepancy" [Kennedy 01, Higdon 04].

$$\xi_{\tilde{\nabla}}(c)_1 = \rho_1 \, \nabla\xi(c)_1 + \epsilon_1(c)$$
$$\cdots$$
$$\xi_{\tilde{\nabla}}(c)_d = \rho_d \, \nabla\xi(c)_d + \epsilon_d(c)$$

$$\xi_{\tilde{\nabla}} : \text{ estimated gradient }, \qquad \nabla\xi : \text{ true gradient }.$$

Assumptions for modeling the gradient

- Model $\xi, \epsilon_1, \cdots, \epsilon_d$ as stationary Gaussian processes with covariances $K, G_1, \cdots, G_d$ respectively [Kennedy 01, Higdon 04] .
- Assume the gradient error to be independent with the objective.

$$\mathrm{cov}\left[\xi(c_1), \epsilon_i(c_2)\right] = 0 \qquad \text{for all } c_1, c_2 \in \mathcal{C}\ .\ i = 1, \cdots, d\ .$$

- For simplicity, assume the components of the gradient error are pairwise independent.

$$\mathrm{cov}\left[\epsilon_i, \epsilon_j\right] = 0 \quad \text{for } i \neq j$$

- For simplicity, assume the covariance functions are isotropic. $K(c_1, c_2),\ G_1(c_1, c_2),\ \cdots\ G_d(c_1, c_2)$ only depend on $\left\|c_1 - c_2\right\|$. (Use L_2 norm.)

Modeling the joint distribution

Predict ξ and its error bar at a new point c using co-Kriging.
$\underline{c}_n := (c_1, \cdots, c_N)$: sampled points.

$$\begin{pmatrix} \xi(c) \\ \xi(\underline{c}_n) \\ \xi_{\tilde{\nabla}}(\underline{c}_n) \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} \mu \\ \boldsymbol{\mu} \\ \mathbf{0} \end{pmatrix}, \begin{pmatrix} K(c,c) & \mathbf{v} & \mathbf{w} \\ \mathbf{v}^T & \mathbf{D} & \mathbf{H} \\ \mathbf{w}^T & \mathbf{H}^T & \mathbf{E}+\mathbf{G} \end{pmatrix} \right),$$

$$\mathbf{v} = (K(c,c_1), \cdots, K(c,c_N)), \quad \mathbf{w} = (\nabla_{c_1} K(c,c_1), \cdots, \nabla_{c_N} K(c,c_N))$$

$$\mathbf{D} = \begin{pmatrix} K(c_1,c_1) & \cdots & K(c_1,c_N) \\ \vdots & \ddots & \vdots \\ K(c_N,c_1) & \cdots & K(c_N,c_N) \end{pmatrix}, \quad \mathbf{H} = \begin{pmatrix} \nabla_{c_1'} K(c_1,c_1') & \cdots & \nabla_{c_N'} K(c_1,c_N') \\ \vdots & \ddots & \vdots \\ \nabla_{c_1'} K(c_N,c_1') & \cdots & \nabla_{c_N'} K(c_N,c_N') \end{pmatrix}$$

$$\mathbf{E} = \begin{pmatrix} \nabla_{c_1}\nabla_{c_1'} K(c_1,c_1') & \cdots & \nabla_{c_1}\nabla_{c_N'} K(c_1,c_N') \\ \vdots & \ddots & \vdots \\ \nabla_{c_1}\nabla_{c_N'} K(c_N,c_1') & \cdots & \nabla_{c_N}\nabla_{c_N'} K(c_N,c_N') \end{pmatrix}, \quad \mathbf{G} = \begin{pmatrix} G(c_1,c_1') & \cdots & G(c_1,c_N') \\ \vdots & \ddots & \vdots \\ G(c_N,c_1') & \cdots & G(c_N,c_N') \end{pmatrix}$$

$$G(c_i,c_j) = \mathrm{diag}\big(G_1(c_i,c_j), \cdots, G_d(c_i,c_j)\big)$$

Determine the hyper-parameters

- The Matern 5/2 kernel [Matern 60, Snoek 12]

$$C_{\frac{5}{2}}(c_1, c_2) = \sigma^2 \left(1 + \frac{\sqrt{5}|c_1 - c_2|}{L} + \frac{5|c_1 - c_2|^2}{3L^2}\right) \exp\left(-\frac{\sqrt{5}|c_1 - c_2|}{L}\right)$$

Hyper-parameters: σ^2's, L's, ρ's, and μ.

- Maximum likelihood estimate (MLE)[Jones 98]

$$\max_{\sigma^2, L, \rho, \mu} \left\{\log p\left(\xi(\underline{c}_n), \xi_{\tilde{\nabla}}(\underline{c}_n) \middle| \sigma^2, L, \rho, \mu\right)\right\}$$

Solved by gradient based optimization.

- Full Bayesian approach [Higdon 04, Kennedy 01]

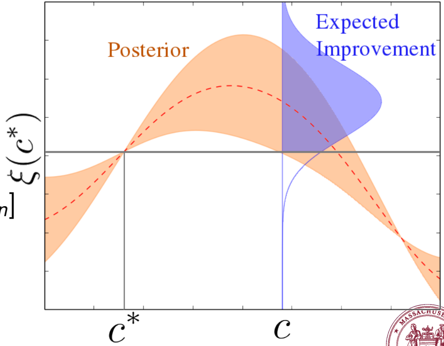
$$p(\sigma^2, L, \rho \,|\, \xi(\underline{c}_n), \xi_{\tilde{\nabla}}(\underline{c}_n))$$

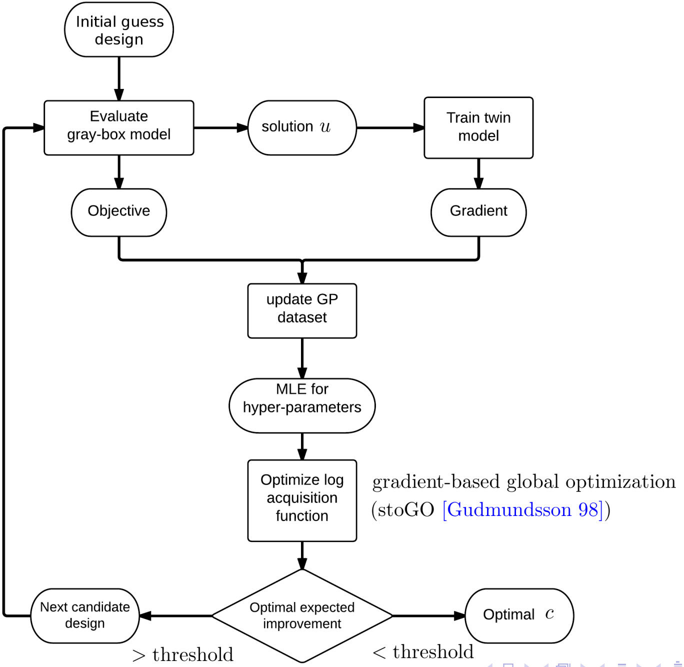
- Both approaches provide similar results [Bayarri 07] . We use the MLE approach.

- GPO introduces an acquisition function:
  $\rho(c)$: the expected utility of investing the next sample at c given the posterior.

- Expected improvement
  [Mokus 78, Snoek 12]

$$\rho_{\mathrm{EI}}(c) = \mathbb{E}\left[\max\left(\xi(c) - \xi(c^*), 0\right) | \mathcal{F}_n\right]$$




Initial guess design
Evaluate gray-box model
solution u
Train twin model
Objective
Gradient
update GP dataset
MLE for hyper-parameters
Optimize log acquisition function
gradient-based global optimization
(stoGO [Gudmundsson 98])
Next candidate design
Optimal expected improvement
Optimal c
$>$ threshold
$<$ threshold

GPO will explore the entire design space as $n \to \infty$. [**Vazquez 10**]

Twin-model GPO will explore the entire design space as $n \to \infty$.

- Let $\xi \in \mathcal{K}(\mathcal{C})$. $\mathcal{K}$ is the reproducing kernel Hilbert space (RKHS) with the semi-positive definite kernel $K : \mathcal{C} \times \mathcal{C} \to \mathbb{R}$. Define $\Phi(c) := K(c, 0)$ for all $c \in \mathcal{C}$. $\hat{\Phi}$ denotes the Fourier transform of Φ.

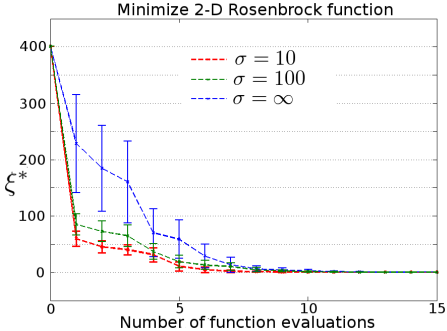
  Let $\epsilon_i \in \mathcal{H}_G^i$. $\mathcal{H}_G^i$ is the RKHS with the semi-positive definite kernel G_i.

- Assume there exist $C \geq 0$ and $k \in \mathbb{N}^+$, such that $(1 + |\eta|^2)^k \left|\hat{\Phi}(\eta)\right| \geq C$ for all $\eta \in \mathbb{R}^d$.

- For all $c_{init} \in \mathcal{C}$, all $\xi \in \mathcal{H}_K$ and $\epsilon_i \in \mathcal{H}_G^i$, $i = 1, \cdots, d$, the sequence c_n generated by twin-model GPO is dense in $\mathcal{C}$.

Gradient improves optimization performance

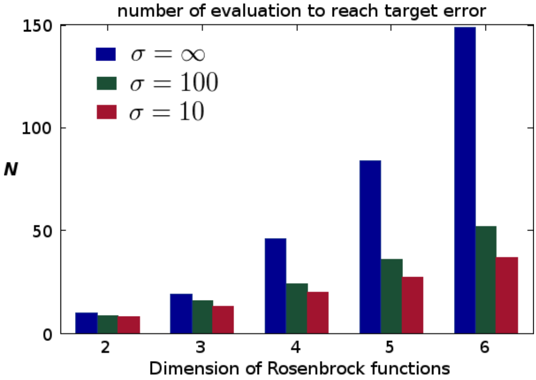
- Rosenbrock 2-D
$$\xi(c_1, c_2) = (1 - c_1)^2 + 100(c_2 - c_1^2)^2$$
Global minimum $\xi(1,1) = 0$
- Simulate $\epsilon_i,\ i = 1, \cdots, d$ by i.i.d. stationary GP with correlation length 1 and variance σ^2.
Accurate: $\sigma = 10$. Noisy: $\sigma = 100$. None: $\sigma = \infty$.



More benefit for higher dimension

- Generalized *n*-D Rosenbrock function

$$\xi(c) = \sum_{i=0}^{d-2} 100(c_{i+1} - c_i)^2 + 1(1 - c_i)^2$$



Outline

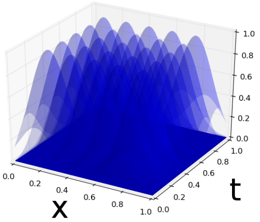
- Background.
- Estimate gradient by using the space(-time) solution.
- Optimization framework.
- Numerical examples

- $u(t, x)$ generated by:

$$\frac{\partial u}{\partial t} + \frac{\partial F(u)}{\partial x} = c(t, x) \quad x \in [0, 1]\ t \in [0, 1]$$
$$u(t = 0, x) = u_0(x),\ u(t, x = 0) = u(t, x = 1)$$

- Control:

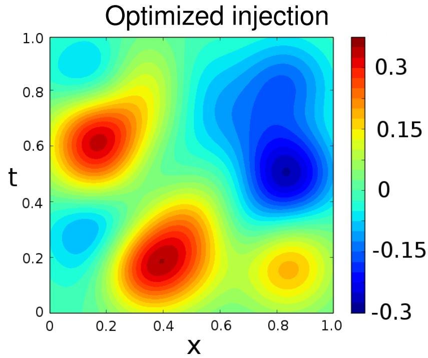
$$c(t, x) = \sum_{i=1}^{m} \sum_{j=n}^{s} c_{ij} \cdot B_{ij}(t, x)$$
$$B_{ij} = \exp\left(-\frac{(t - t_i)^2}{L_t^2}\right) \exp\left(-\frac{(x - x_j)^2}{L_x^2}\right)$$

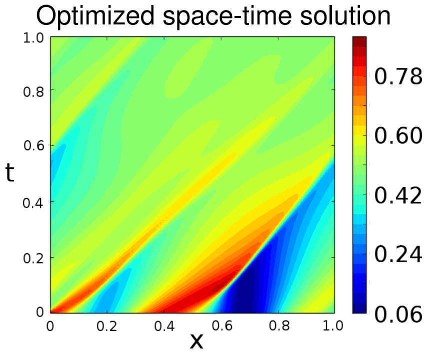


- Objective function:

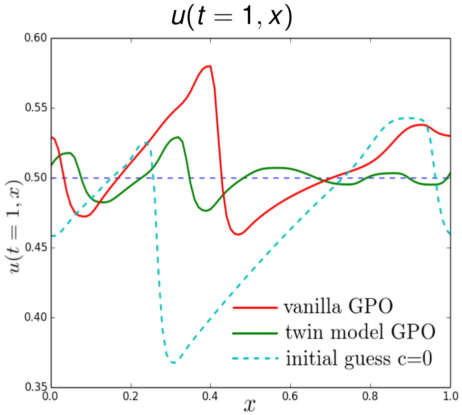
$$\xi(c) = \int_{x=0}^{1} \left| u(t = 1, x) - \frac{1}{2} \right|^2 + \lambda \sum_{ij} c_{ij}^2, \quad \lambda > 0$$

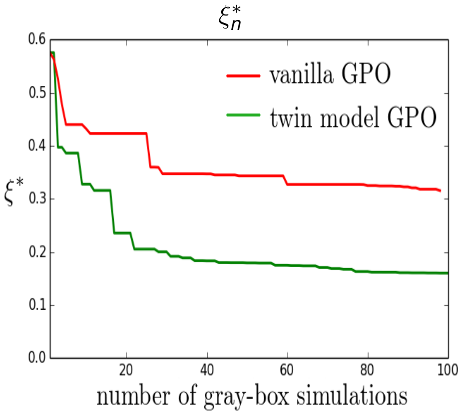
Optimized injection





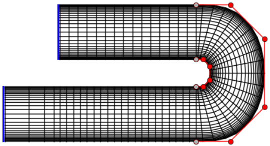
Compare optimization performance

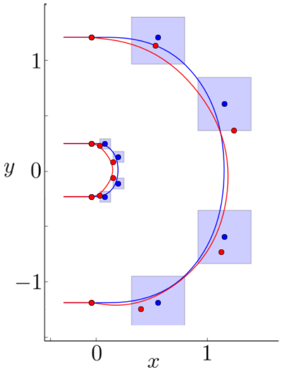


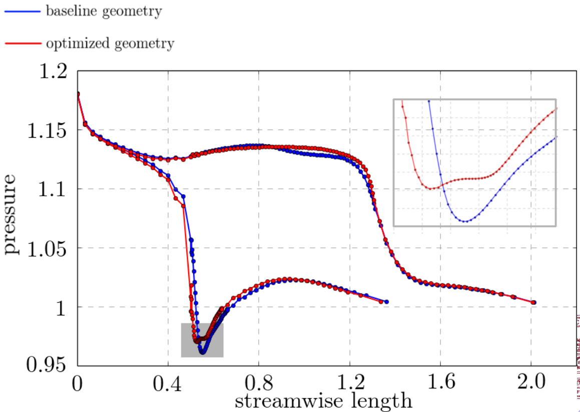


Optimize return bend

Objective: maximize mass flux.
Constraint by fixed area of the return bend.
Unknown state equation.

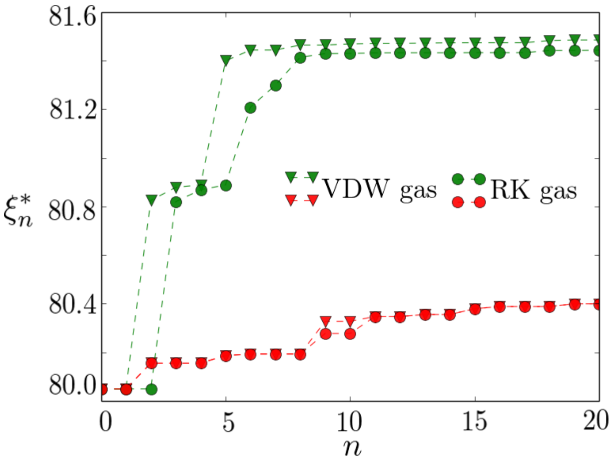






Twin model improves GPO performance

- Faster improvement for the current best objective function evaluation.
- Most improvement is achieved for small *n*.



Conclusions

- Developed the twin model method to efficiently estimate the gradient of objective functions constrained by gray-box simulations.
- Practically and theoretically demonstrated the utility of the estimated gradient in a Bayesian optimization framework.
- Applied the twin-model GPO to a Buckley-Leverett simulation and the Navier-Stokes simulaiton to reduce the number of gray-box simulations required to achieve desired optimization results.

Enjoy the spring break!

Details of return bend testcase

N-S equation:

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho\\ \rho u\\ \rho v\\ \rho E\end{pmatrix}+\frac{\partial}{\partial x}\begin{pmatrix}\rho u\\ \rho u^2+p-\sigma_{xx}\\ \rho uv-\sigma_{xy}\\ u(E\rho+p)-\sigma_{xx}u-\sigma_{xy}v\end{pmatrix}+\frac{\partial}{\partial y}\begin{pmatrix}\rho v\\ \rho uv-\sigma_{xy}\\ \rho v^2+p-\sigma_{yy}\\ v(E\rho+p)-\sigma_{xy}u-\sigma_{yy}v\end{pmatrix}=\mathbf{0}$$

where

$$\sigma_{xx}=\mu\left(2\frac{\partial u}{\partial x}-\frac{2}{3}\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}\right)\right)$$

$$\sigma_{yy}=\mu\left(2\frac{\partial v}{\partial y}-\frac{2}{3}\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}\right)\right)$$

$$\sigma_{xy}=\mu\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)$$

$$p_{\text{ideal}}=(\gamma-1)U$$

$$p_{\text{vdw}}=\frac{(\gamma-1)U}{1-b_{vdw}\rho}-a_{vdw}\rho^2$$

$$p_{\text{rk}}=\frac{(\gamma-1)U}{1-b_{rk}\rho}-\frac{a_{rk}\rho^{5/2}}{((\gamma-1)U)^{1/2}(1+b_{rk}\rho)}$$

Inlet: $\rho,\ p_t=p\left(1+\frac{1}{5}M^2\right)^{3.5}$ fixed.

Outlet: p fixed.

Approximation by superposition of sigmoids

The sigmoid functions can form the bases for continuous $f : \mathbb{R}^d \to \mathbb{R}$.

- [Mhaskar 92] has shown that: for any integer $s \geq 1$, any compact set $\Omega \subset \mathbb{R}^d$, any continuous function $f : \Omega \to \mathbb{R}$, and any $\epsilon > 0$, there exist an integer N, numbers $\alpha_k, t_k \in \mathbb{R}$ and $\lambda_k \in \mathbb{R}^d$, such that

$$\sup_{x\in\Omega} \left| f(x) - \sum_{k=1}^{N} \alpha_k \phi(\lambda_k \cdot (x - t_k)) \right| < \epsilon$$

- If $v_1, \cdots, v_n$ is a basis for V, $w_1, \cdots, w_m$ is a basis for W, then $\{v_i \otimes w_j\}_{1\leq i\leq n, 1\leq j\leq m}$ is a basis for $V \otimes W$.
  The theorem also holds for infinite dimensional V, W.

Accuracy of gradient estimation

- What flow quantity to use to compute $\mathcal{M}$? (Goal-oriented approach?)
- How to quantify $\mathcal{M}$ and estimation error in $\frac{d\xi}{dc}$?
  - Consider a special case

$$\frac{\partial u}{\partial t} + \nabla \cdot F(u) = c\,, \quad \frac{\partial \tilde{u}}{\partial t} + \nabla \cdot \tilde{F}(\tilde{u}) = c\,, \qquad \tilde{F} = F + \delta F$$

with $u\big|_{t=0} = u_0$ and $\frac{\partial u}{\partial \mathbf{n}}\big|_{\partial\Omega} = 0$.

$$\text{Objective:} \quad \xi = \int_t \int_\Omega g(u) dxdt$$

  - After linearization, the solution error δu and the adjoint error δv satisfy

$$\frac{\partial \delta u}{\partial t} + \nabla \cdot \left(\frac{dF}{du} \delta u \right) = -\nabla \cdot \delta F$$

$$\frac{\partial \delta v}{\partial t} + \frac{dF}{du} \cdot \nabla \delta v = -\frac{d^2 g}{du^2} \delta u - \frac{d\delta F}{du} \cdot \nabla v - \frac{d^2 F}{du^2} \cdot \nabla v \delta u$$

Non-stationary GP modeling

- Non-stationary covariance functions allow GP to adapt to functions whose smoothness varies with the inputs.
- $$K^{NS}(c_i, c_j) = \int k_{c_i}(c) k_{c_j}(c) dc$$

  For Gaussian kernels [Higdon 99] ,

  $$K^{NS}(c_i, c_j) = \sigma^2 |\Sigma_i|^{1/4} |\Sigma_j|^{1/4} \left| (\Sigma_i + \Sigma_j) / 2 \right|^{-1/2} \exp(-Q_{ij})$$

  $$Q_{ij} = (c_i - c_j)^T \left((\Sigma_i + \Sigma_j)/2 \right)^{-1} (c_i - c_j)$$
- The extension of GP to non-stationary introduces additional parameterization that models the variation of the kernel.

Reduce computational cost of GPO

- The search of the next candidate design requires optimizing an acquisition function.
- Requires repetitive evaluation of

$$(\mathbf{v},\mathbf{w})\underbrace{\begin{pmatrix}\mathbf{D} & \mathbf{H}\\ \mathbf{H}^T & \mathbf{E}+\mathbf{G}\end{pmatrix}^{-1}}_{\Sigma}(\mathbf{v},\mathbf{w})^T$$

  for different c. $\Sigma : n(d+1)\times n(d+1)$.
- Cholesky decomposition $\Sigma = \mathbf{L}\mathbf{L}^T$, $\mathcal{O}(n^3(d+1)^3)$ FLOPs.
- The inclusion of new data at $c = c'$ updates $\mathbf{L}$ by

$$\mathbf{L}_{\text{updated}} \leftarrow \begin{pmatrix}\mathbf{L} & \lambda^T\\ \lambda & K(c',c') - \lambda^T\lambda\end{pmatrix}\,, \quad \lambda = (\mathbf{v},\mathbf{w})\mathbf{L}^{-T}$$

  Updating the Cholesky decomposition requires $\mathcal{O}(n^2(d+1)^2)$ FLOPs.
- Sparse GP is also applicable (e.g. greedy subset selection [Smola 01], latent variable method [Lawrence 04]), at the cost of reducing accuracy.

Reduce computational cost of twin model

- Instead of minimizing the solution mismatch $\mathcal{M}$, we can minimize

$$\mathcal{R} := \int_t \int_x \left\| \tilde{R}(u) \right\| dxdt\,, \qquad \tilde{R}(u) = \dot{u} + \nabla \cdot \tilde{F}(u) - q(u, c)\,,$$

  thus avoid the integration of twin model PDE.

- Small residual does not guarantee small solution mismatch.
  - Consider the discretized the gray-box and twin models:

$$\begin{aligned} \text{twin model: } \tilde{u}_{t+1} - \mathcal{G}\tilde{u}_t = 0 \\ \text{gray-box model: } u_{t+1} - \mathcal{H}u_t = 0 \end{aligned}\,, \qquad t = 0, \cdots, T-1$$

$$\tilde{R}(u) \approx \left\| u_1 - \mathcal{G}u_0 \right\|^2 + \cdots \left\| u_T - \mathcal{G}u_{T-1} \right\|^2$$

  If $\|\mathcal{G}u - \mathcal{G}u'\| \leq \alpha \|u - u'\|$ for all u, u' with $\alpha < 1$, then $\mathcal{M} \leq \frac{1}{1-\alpha}\mathcal{R}$.

- We first minimize the residual, then minimize the solution mismatch. The procedure reduces the cost of training, and yields good twin model.

- Constraints independent of u,

$$\text{e.g.} \quad \boldsymbol{c}_{\text{lower}} \le \boldsymbol{c} \le \boldsymbol{c}_{\text{upper}}$$

Enforced in optimizing $\rho(c|\mathcal{F}_n)$.

- Constraints depends on u
  - Modify the objective function
    e.g. penalty methods[Homaifar 94] , augmented lagrangian methods [Conn 91], barrier function methods [Conn 97].
  - Modify the acquisition
    e.g. expected improvement with constraints (EIC [Gardner 14])

$$\mathbb{E}\left[\max(\xi(c) - \xi(c_n^*), 0)\middle|\mathcal{F}_n\right] \mathbb{P}\left[g(c) \le 0\right]$$

integrated expected conditional improvement (IECI [Gramacy 11]).

$$\int_{\mathcal{C}} \left[\rho\left(c'\right) - \rho\left(c'\middle|c\right)\right] \mathbb{P}[g(c) \le 0] \, \mathrm{d}c'$$

Analyze computational cost: twin model

n: num of gray-box simulations.
n_b: average num of basis addition / deletion.
$n_{\mathcal{M}}$: average num of twin model simulations to minimize $\mathcal{M}$.
d: $\dim(c)$.
C_T: cost of running the twin model for once.
C_G: cost of running the gray-box model for once.

- Cost for training twin model at each design c
  - Twin model may offer significant benefit if

$$\frac{C_T}{C_G} < \frac{d}{n_b n_{\mathcal{M}}}$$

  - Reuse trained twin model to reduce n_b, $n_{\mathcal{M}}$.
  - Reduce C_T by minimizing the twin model residual's first.

Analyze computational cost: GPO

n: num of gray-box simulations.
d: $\dim(c)$.
n_ρ: average num of ρ evalutions for each max ρ.
n_{MLE}: average num of likelihood evalutions for each max MLE.

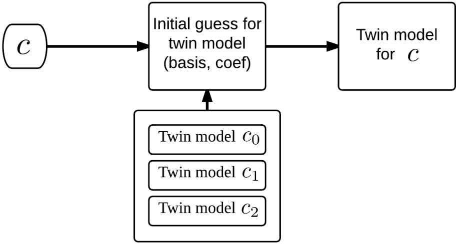
- Cost for MLE and optimizing $\rho(c|\mathcal{F}_n)$ in GPO
  - Cost of likelihood evalution is $\mathcal{O}(n^3 d^3)$.
  - Cost of ρ evaluation is $\mathcal{O}(n^2 d^2)$.
  - Total cost:

$$n\left(\underbrace{n_{MLE}\, n^3 d^3}_{\text{MLE cost}} + \underbrace{n_\rho n^2 d^2}_{\text{max } \rho \text{ cost}}\right)$$

  - MLE cost can be controlled by
    - Use full Bayesian approach [Kennedy 01, Snoek 12] (MCMC).
    - Only update hyper-parameters when determined necessary. Future work.
  - Assume GPO cost negligible vs gray-box simulation cost.

Reuse gray-box solutions and trained twin models backup

- Use previously trained twin model as an initial guess.



  - Search for a design in the trained database which is “closest” to c. Prune the model using the backward steps.
  - More efficient reuse of twin models remains a future work.
- Use multiple solutons to train a single twin model.
  - Incorporate multiple solutions to calibrate a model can improve the predictive performance of the calibrated model. [Arendt 12]
  - In the adjoint analysis, however, $\frac{\partial \xi}{\partial c}$ at a design c only involves $u(c)$.

Prove the search sequence is dense

Lemma (Chapter 1, Theorem 4.1, [Berlinet 11])
Let K_1, K_2 be the reproducing kernels of functions on $\mathcal{C}$ with norms $\|\cdot\|_{\mathcal{H}_1}$ and $\|\cdot\|_{\mathcal{H}_2}$ respectively. Then $K = K_1 + K_2$ is the reproducing kernel of the space

$$\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2 = \{f = f_1 + f_2,\ f_1 \in \mathcal{H}_1,\ f_2 \in \mathcal{H}_2\}$$

with norm $\|\cdot\|_{\mathcal{H}}$ defined by

$$\forall f \in \mathcal{H} \quad \|f\|^2_{\mathcal{H}} = \min_{f=f_1+f_2,\ f_1\in\mathcal{H}_1, f_2\in\mathcal{H}_2} \left(\|f_1\|_{\mathcal{H}_1^2} + \|f_2\|^2_{\mathcal{H}_2}\right)$$

Theorem 1 (Cauchy inequality)

Let $\xi \in \mathcal{K}(\mathcal{C})$. $\mathcal{K}$ is the reproducing kernel Hilbert space (RKHS) with the semi-positive definite kernel $K : \mathcal{C} \times \mathcal{C} \to \mathbb{R}$.

Let $\epsilon_i \in \mathcal{H}^i_G$. $\mathcal{H}^i_G$ is the RKHS with the semi-positive definite kernel G_i.

$$\left|\xi(c, \omega_\xi) - \hat{\xi}(c; \underline{c}_n)\right|^2 \leq C\sigma^2(c; \underline{c}_n)$$

$$C = \left(1 + \frac{4d}{3}\right) \left\|\xi(c; \omega_\xi)\right\|_{\mathcal{H}_K} + \frac{4d}{3} \left\|\nabla_c \xi(c; \omega_\xi)\right\|_{\mathcal{H}_{K_\nabla}} + \frac{4}{3} \sum_{i=1}^{d} \left\|\epsilon_i(c; \omega^i_\epsilon)\right\|_{\mathcal{H}^i_G}$$

Prove the search sequence is dense, cont.

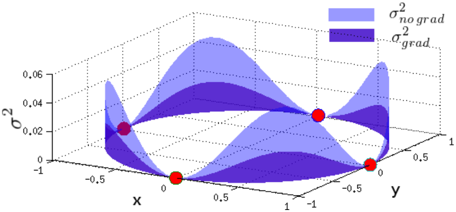
Theorem 2 Let $(\underline{c}_n)_{n\geq 1}$ and $(\underline{a}_n)_{n\geq 1}$ be two sequences in $\mathcal{C}$. Assume that the sequence (a_n) is convergent, and denote by a^* its limit. Then each of the following conditions implies the next one:
1. a^* is an adherent point of $\underline{c}_n$ (there exists a subsequence in $\underline{c}_n$ that converges to a^*) ,
2. $\sigma^2(a_n; \underline{c}_n) \to 0$ when $n \to \infty$,
3. $\hat{\xi}(a_n; \underline{c}_n) \to \xi(a^*, \omega)$ when $n \to \infty$, for all $\xi \in \mathcal{H}_K$, $\epsilon \in \mathcal{H}_G$.

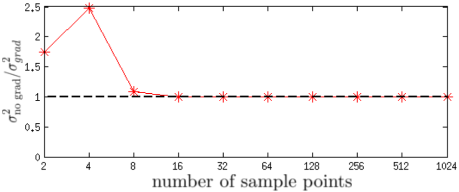
The proof of theorem 2 is similar to the proof of proposition 8 in [Vazquez 10].

Theorem 3 Under the assumption
There exist $C \geq 0$ and $k \in \mathbb{N}^+$, such that $(1 + |\eta|^2)^k \left|\hat{\Phi}(\eta)\right| \geq C$ for all $\eta \in \mathbb{R}^d$.
We have (E. Vazquez, Theorem 5 [Vazquez 10])
If the 3 conditions in Theorem 2 are equivalent, then for all $c_{init} \in \mathcal{C}$ and all $\omega \in \mathcal{H}$, the sequence $\underline{c}_n$ generated by the GP-EI algorithm is dense in $\mathcal{C}$.

Conjecture: convergence rate

- Only the objective value: GPO converges at rate $n^{-\frac{\nu}{d}}$ for ξ in the RKHS associated with Matern ν kernel. [Bull 11].
- Conjecture: Twin-model GPO converges at the same rate as vanilla GPO
  - 1-D Periodic GP $\xi(c)$, $c \in [-\pi, \pi]$
  - Sample uniformly: (1) ξ (2) ξ and noisy $\frac{d\xi}{dc}$.
  - Posteriors becomes indistinguishable as $n \to \infty$.





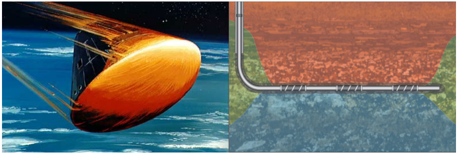
- Twin model boosts optimization in an initial phase of GPO. The boost diminishes as $n \to \infty$.

What if twin model fails?

- Twin model may yield low-quality gradient estimation
  - Gray-box solution is poorly resolved.
  - Wrong conditions used in twin model.
    e.g. wrong I.C. B.C., source term.
  - ...
- We do NOT expect good gradient estimate when assumptions are violated.
- Twin model searches for a model within its model scope to best match the solution.
- The error can be catched by the model discrepancy.
- Worst case scenario: degenerates to derivative-free GPO.

Unknown flux / source / B.C.

- Unknown flux is a common problem:
  - Re-entry vehicle control.
  - Oil reservoir wells / B.C.



- My work is to demonstrate the value of PDE solution in inferring the adjoint.
- Future work to explore the applicability of twin model to unknown source / B.C.

Parallel twin-model GPO

- Parallel Bayesian optimization [Snoek 12] . N evaluations completed, $\{c_i, \xi_i, \xi_{\tilde{\nabla}}\}_{i=1}^{N}$.
  Running gray-box and twin model on J processes, pending data $\{c_j, \xi_j, \xi_{\tilde{\nabla}}\}_{j=1}^{J}$.
  Expected acquisition:

$$\rho(c; \{c_i, \xi_i, \xi_{\tilde{\nabla}}\}_{i=1}^{N}, \{c_j\}_{j=1}^{J}) = \int \rho(c; \{c_i, \xi_i, \xi_{\tilde{\nabla}}\}_{i=1}^{N}, \{c_j, \xi_j, \xi_{\tilde{\nabla}}\}_{j=1}^{J}) d\boldsymbol{\xi} d\boldsymbol{\xi}_{\tilde{\nabla}}$$

- Parallel twin model:
  Twin model is a conservation law simulator that may be parallelled.

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