

From HeartSteps to HeartBeats: Personalized Decision-making



Raaz Dwivedi



HARVARD
UNIVERSITY



Massachusetts
Institute of
Technology

Stanford University, OIT Seminar, Jan 25



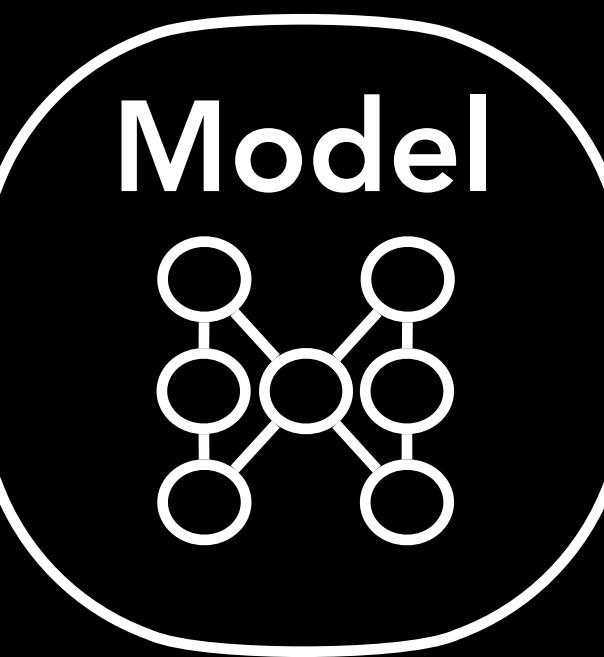
Personalized Decision-making

research & talk overview

Personalized Decision-making

Driven by
extensive data collection,
decreasing cost of computation,
synergy between disciplines

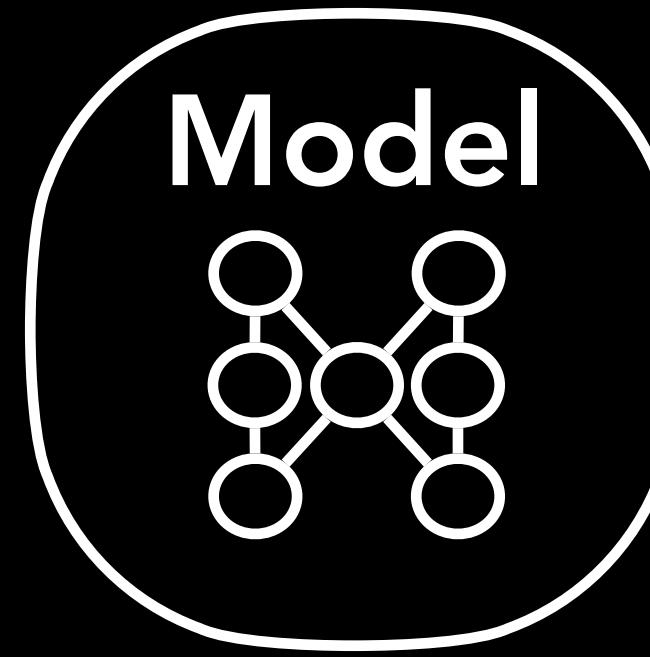
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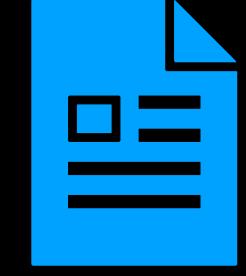
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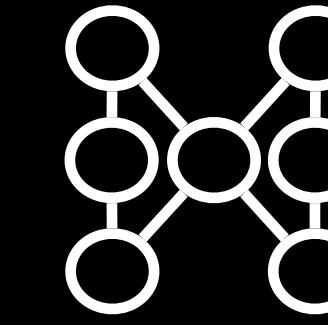
Medical records

Observational
studies

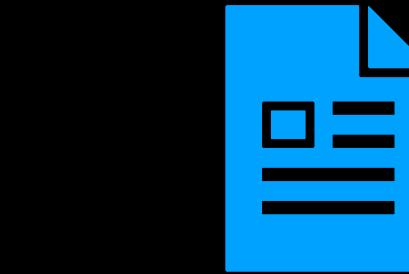


Personalized Decision-making

Model



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Medical records

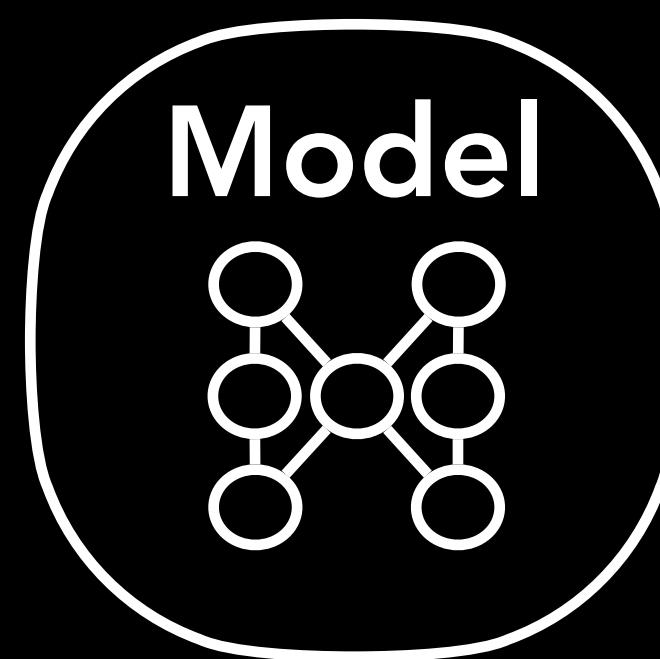
Observational
studies

Drug trial

Randomized
experiments



Personalized Decision-making



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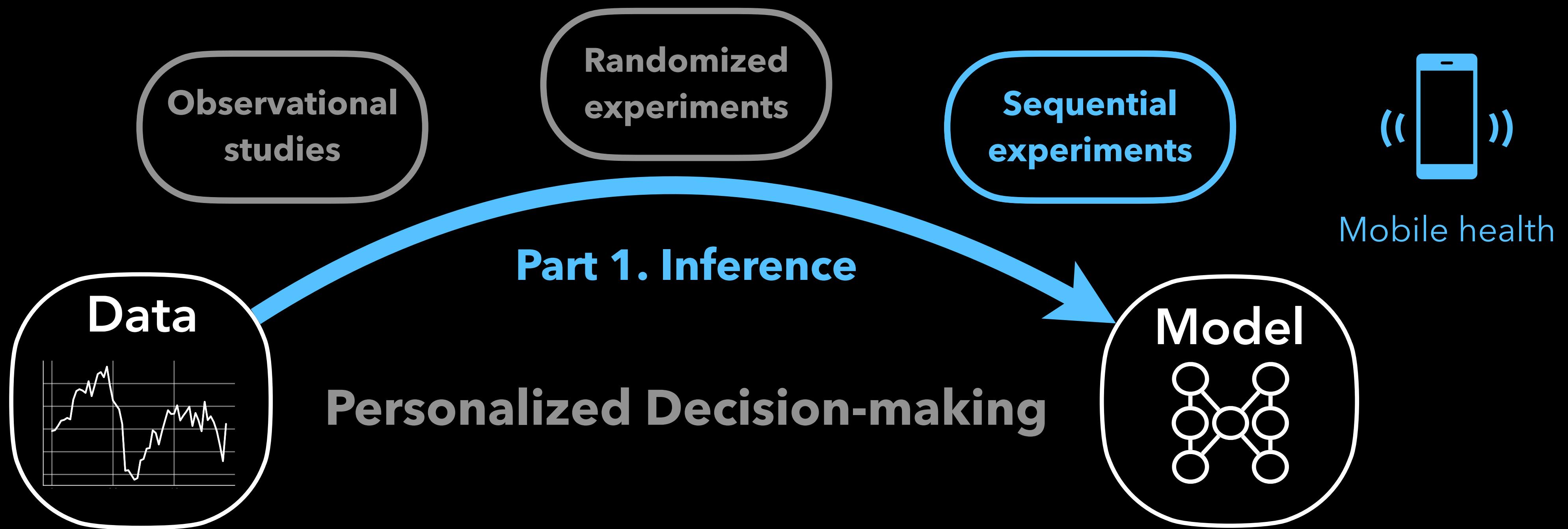
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1. Use **real data** to infer decision's effect

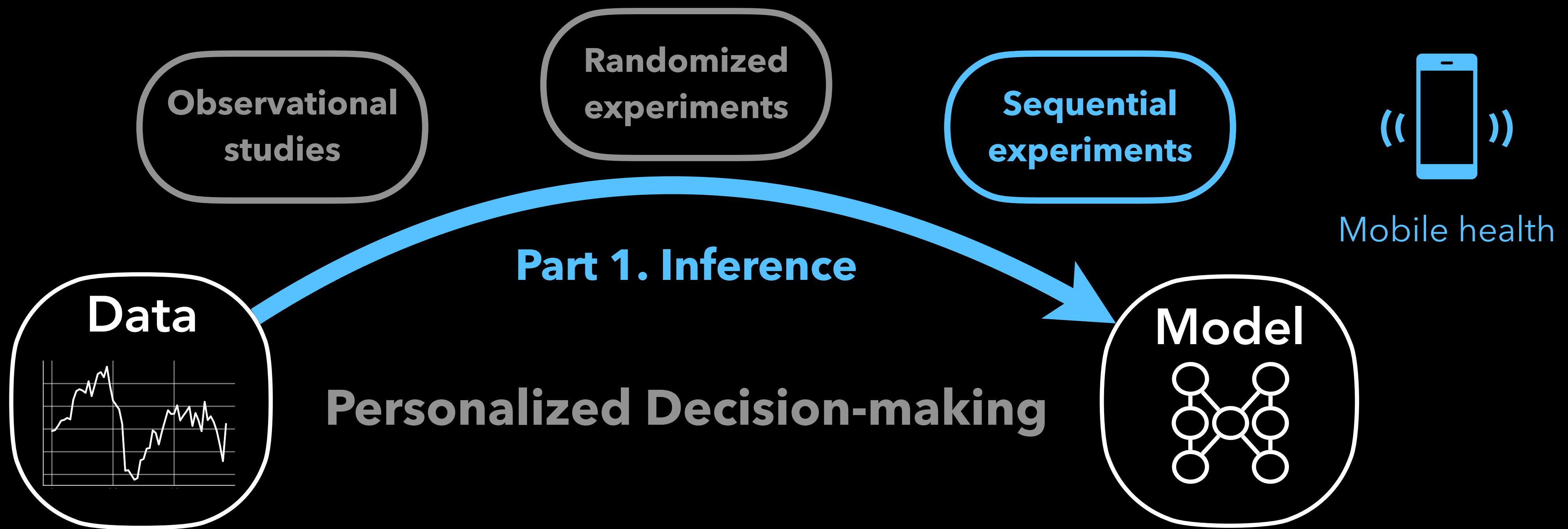


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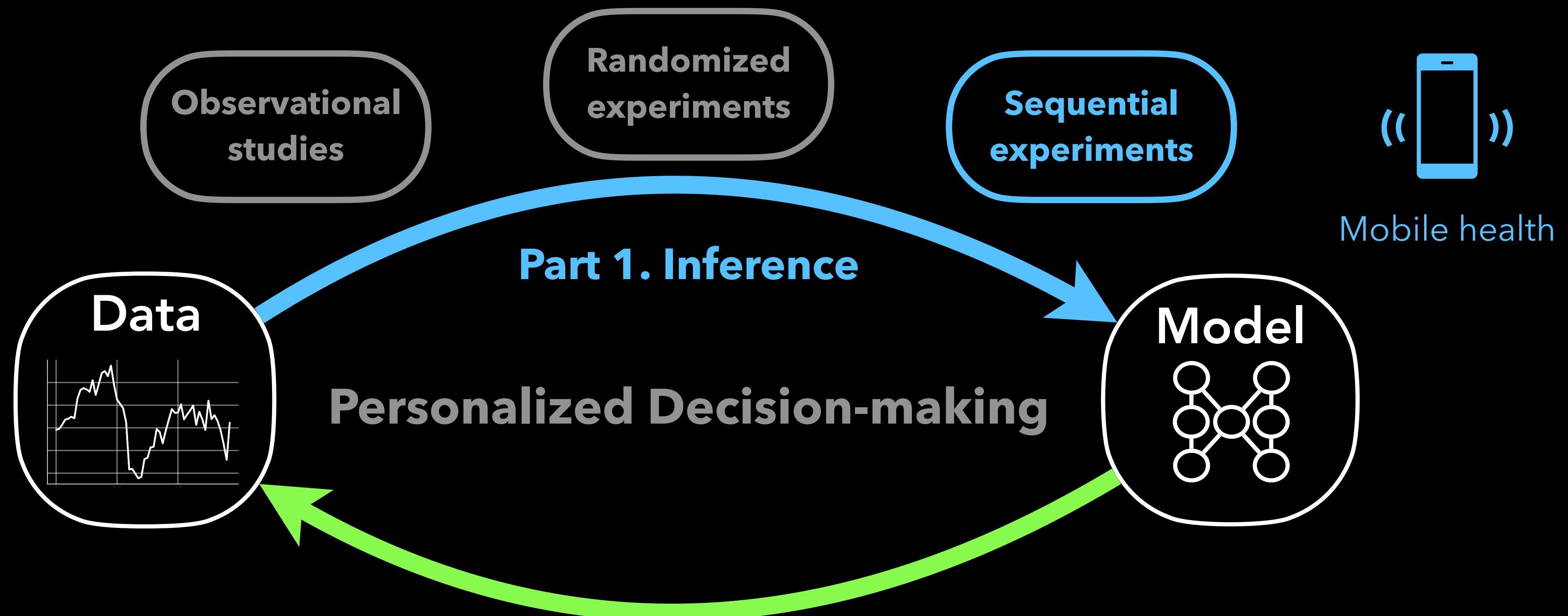
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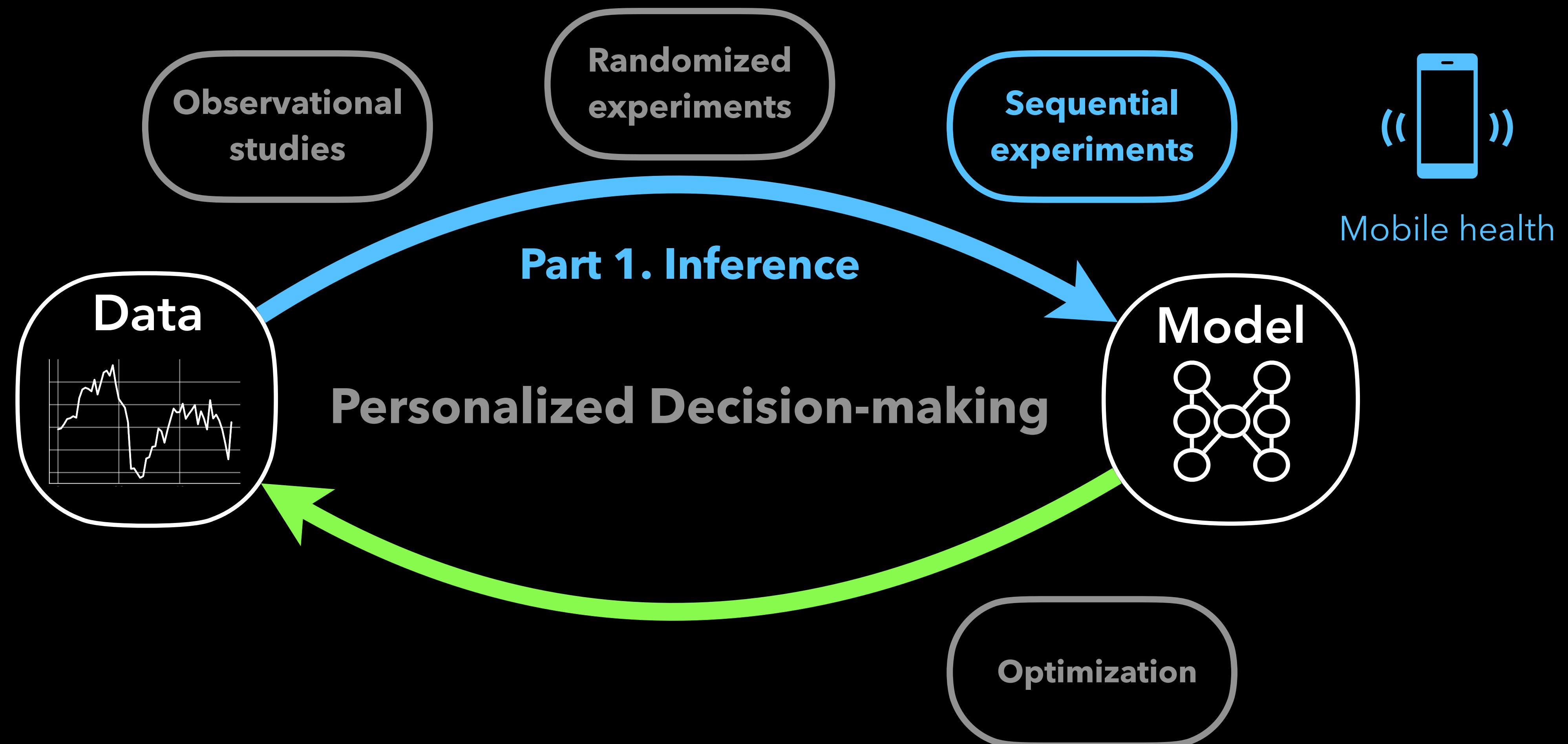
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2. Use **simulated data** to predict decision's effect

research & talk overview

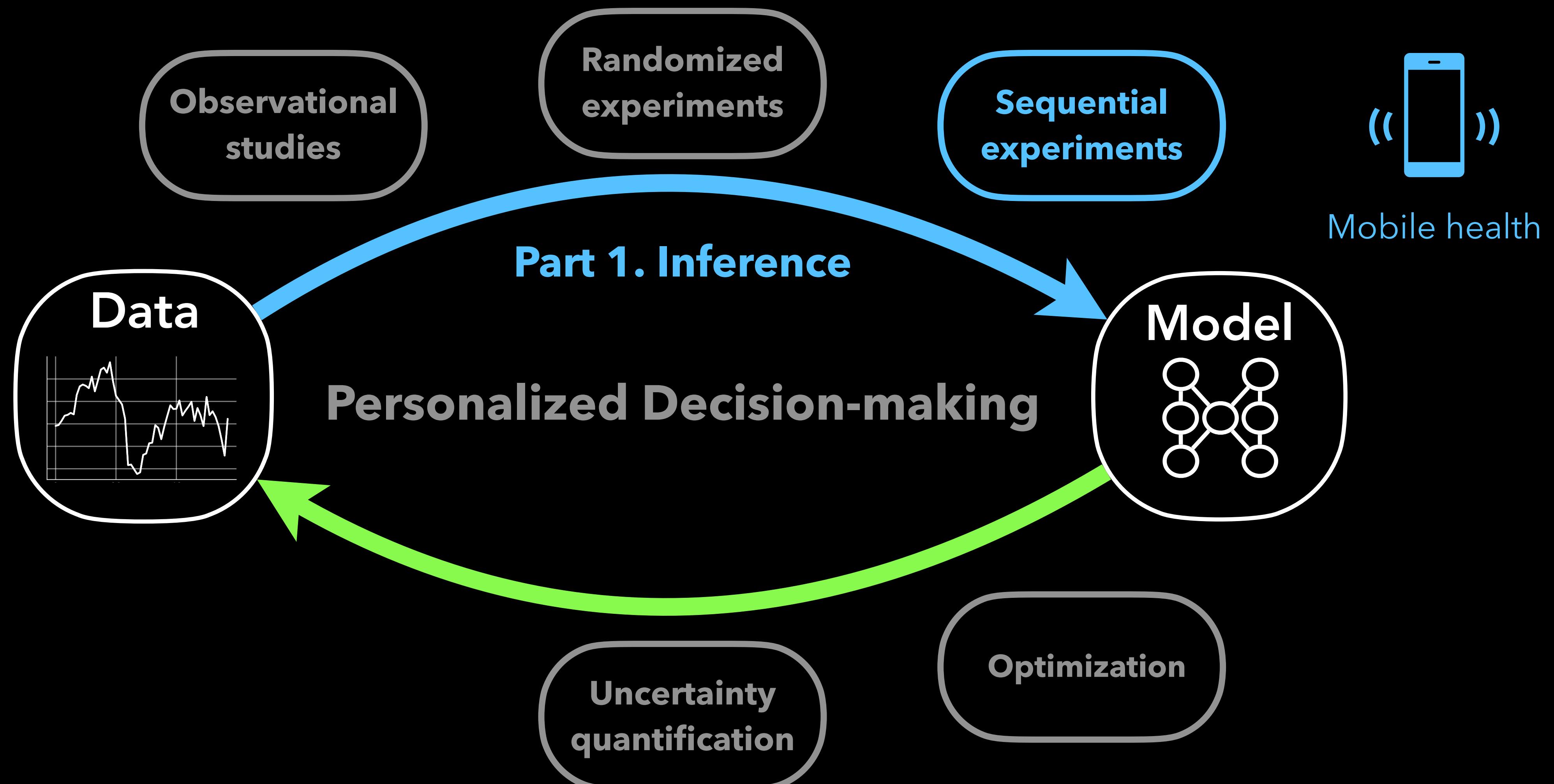
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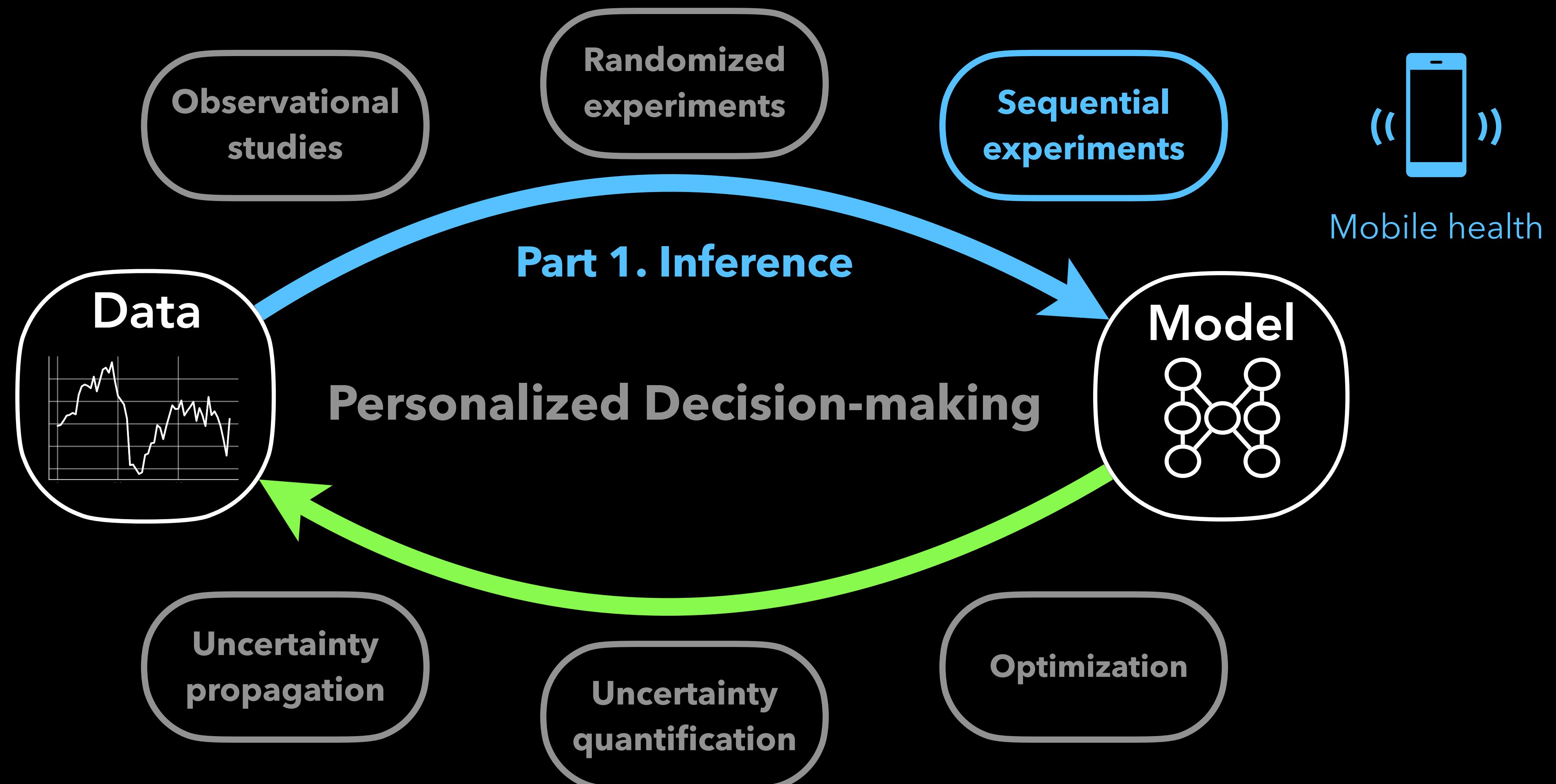
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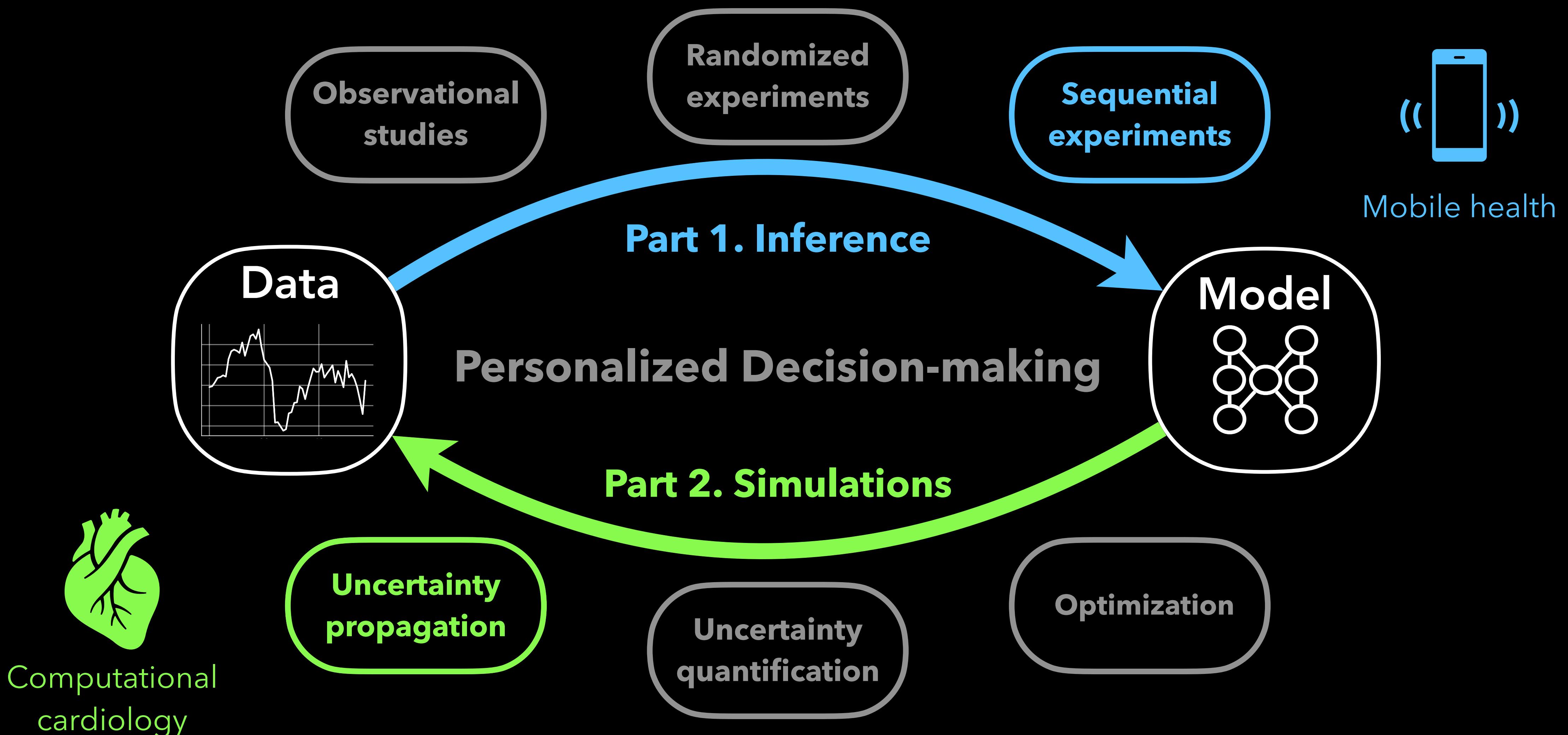
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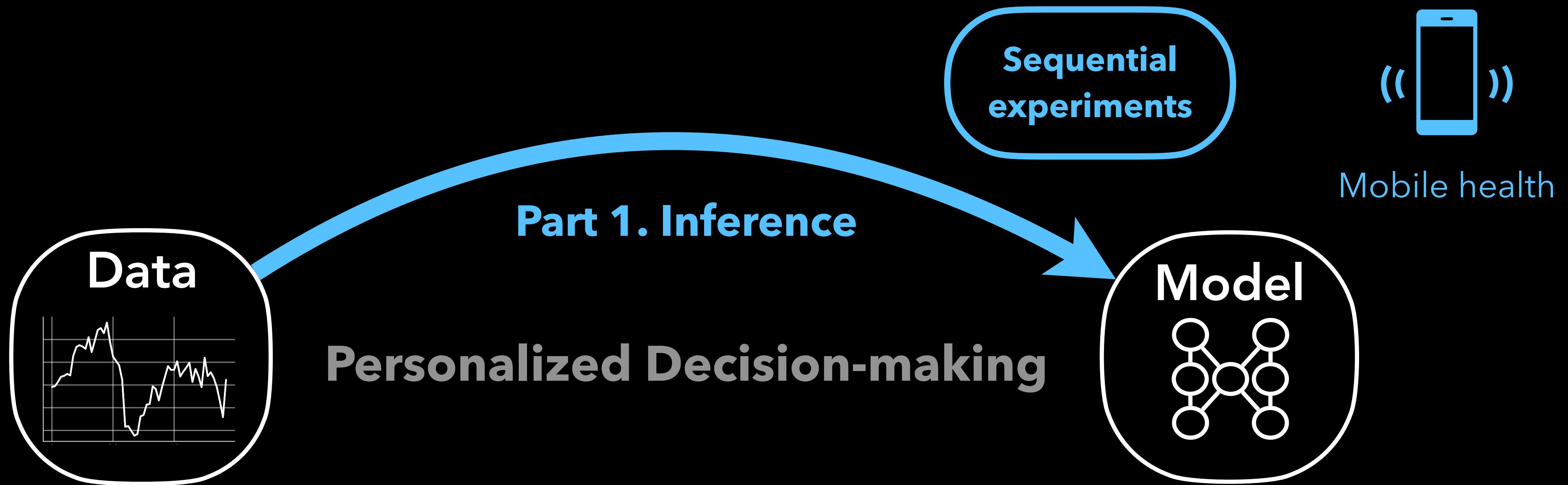
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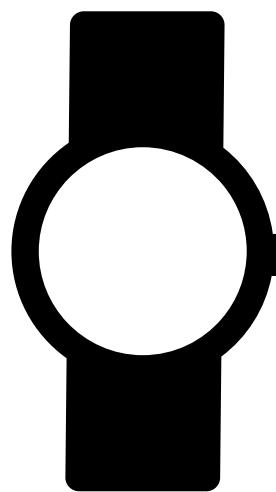
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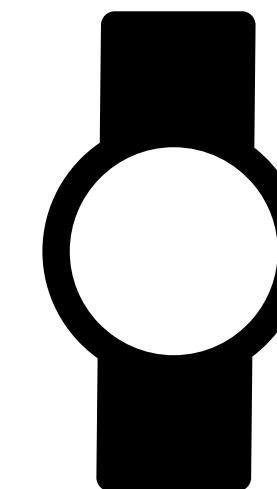
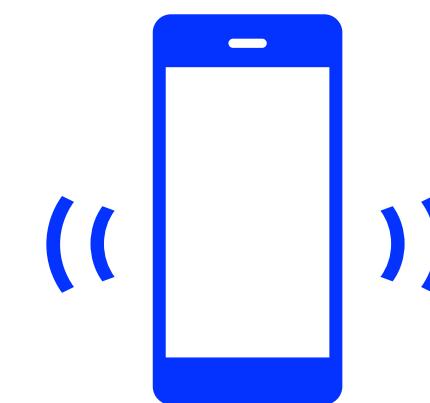


Building AI agents for personalized treatments



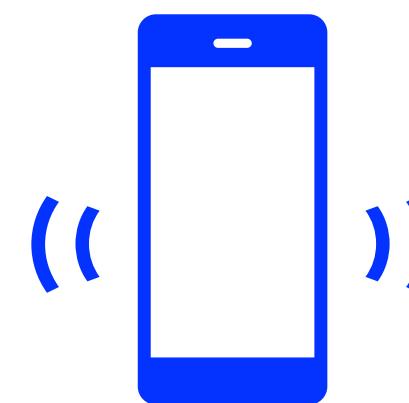
Building AI agents for personalized treatments

How to assign personalized digital
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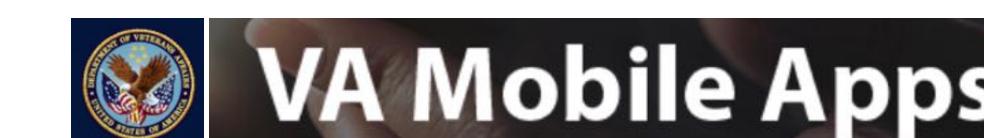
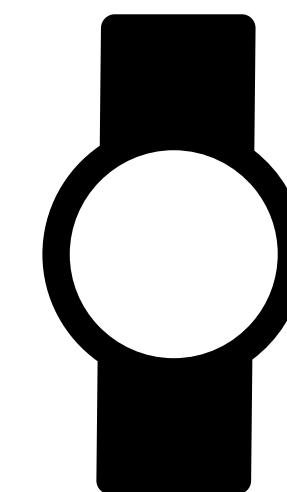
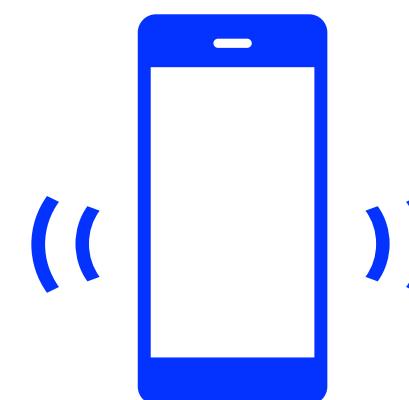


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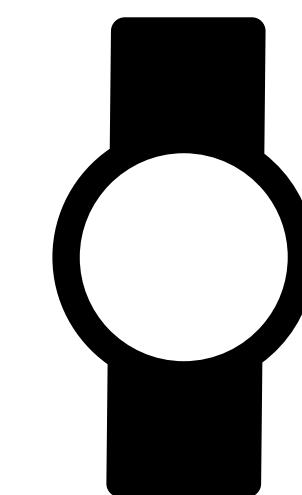


Apple Research app

The future of health research is you.

Building AI agents for personalized treatments

How to assign personalized digital treatments to help you?



Mobile health study:
Personalized HeartSteps

[Liao+ '20]

- ▶ **Goal:** Promote physical activity via mobile app
- ▶ **Population:** 91 hypertension patients, 90 days

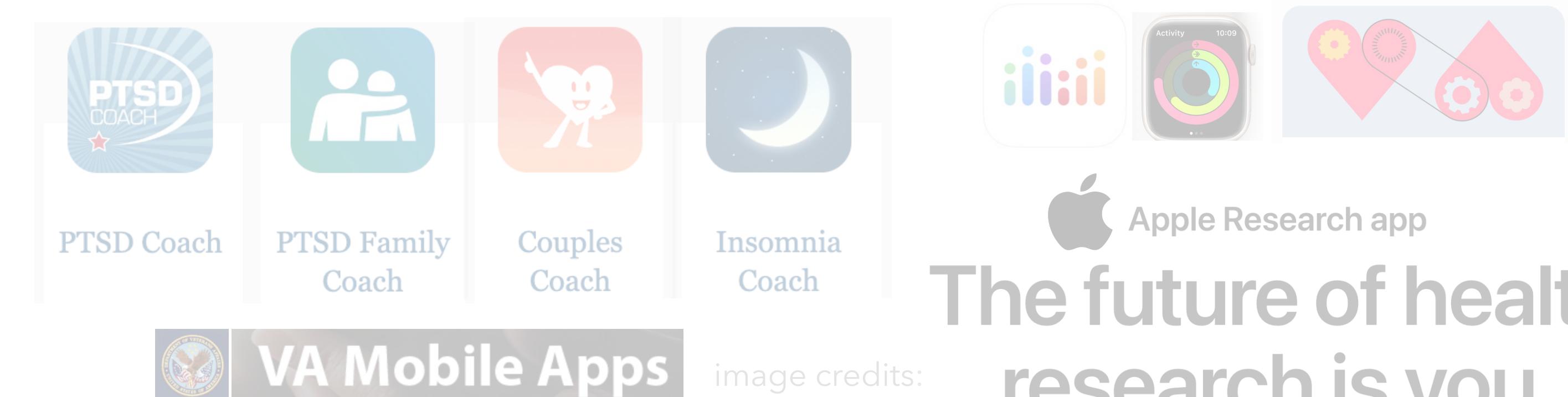
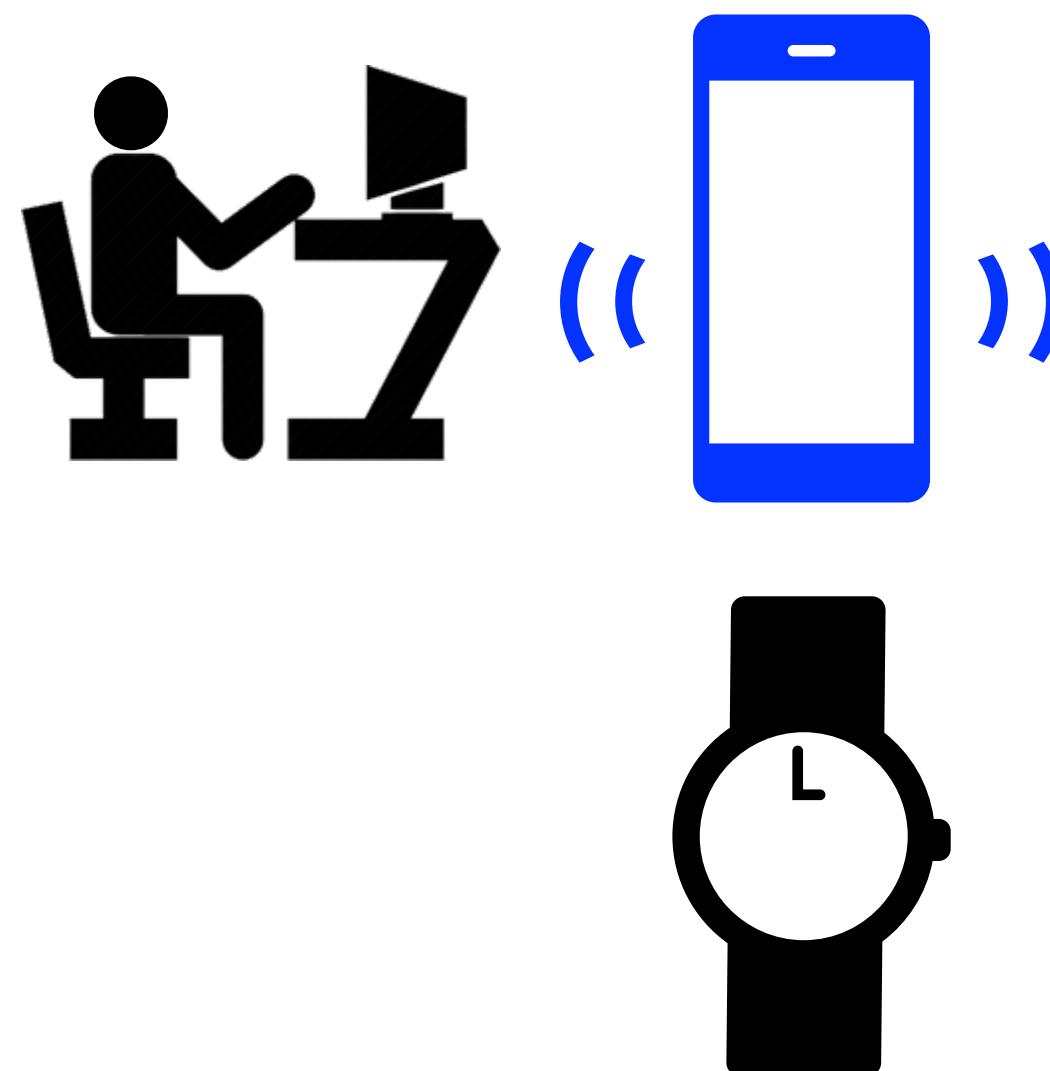


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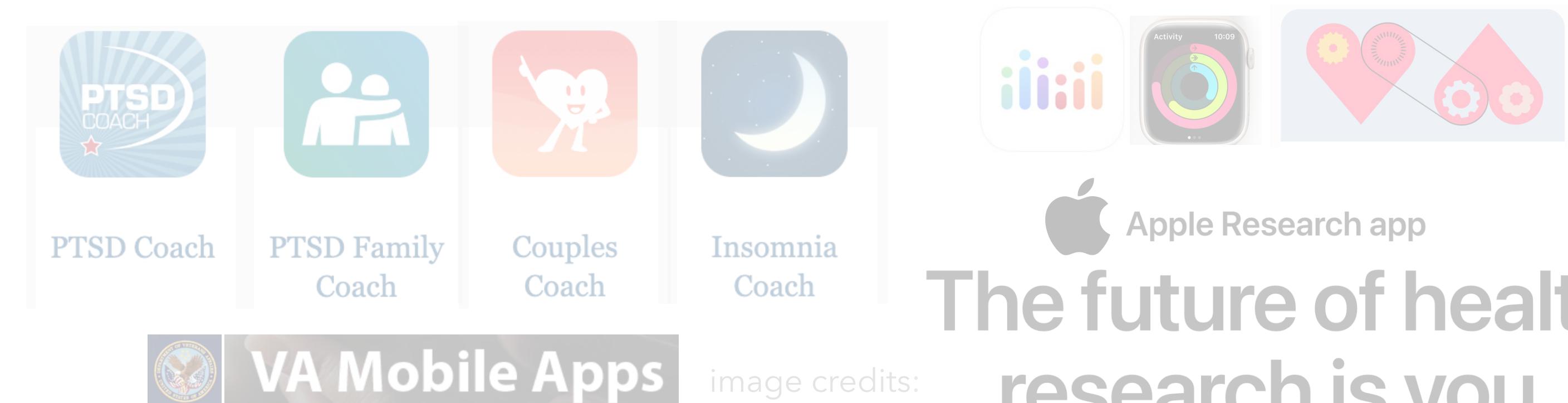
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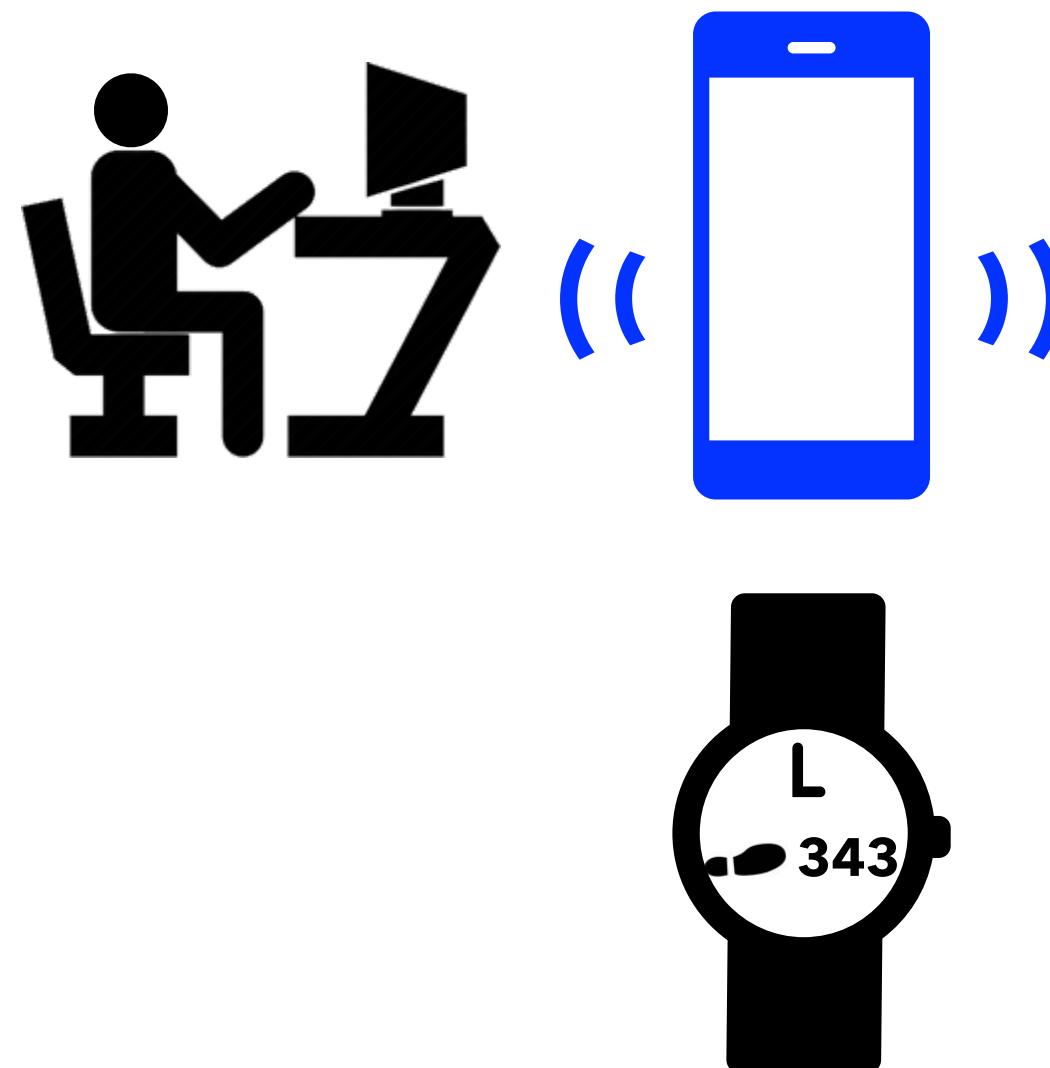
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- ▶ **Outcome:** 30-min step count after decision time

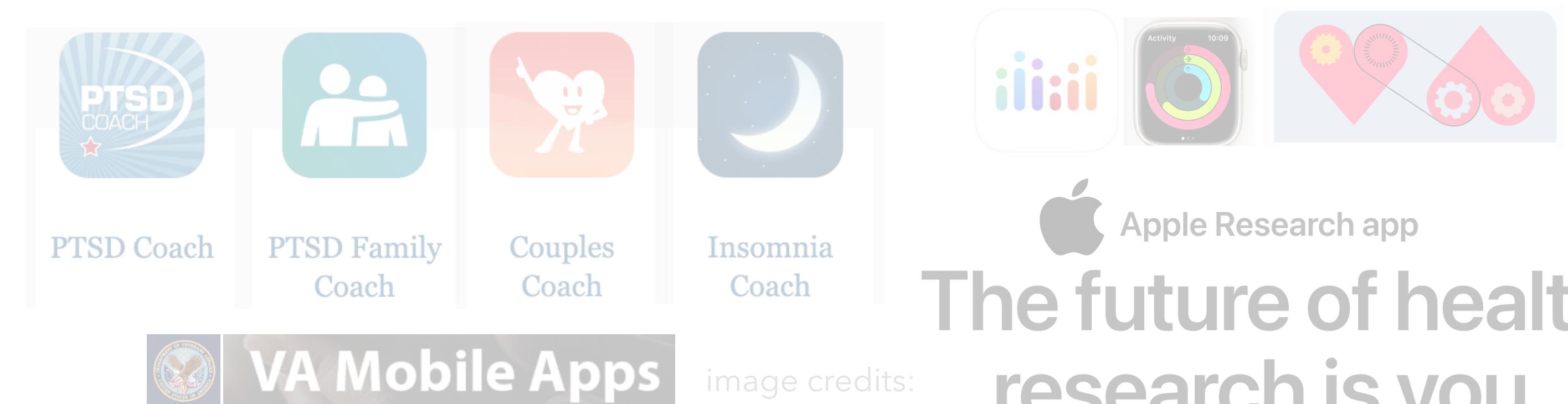
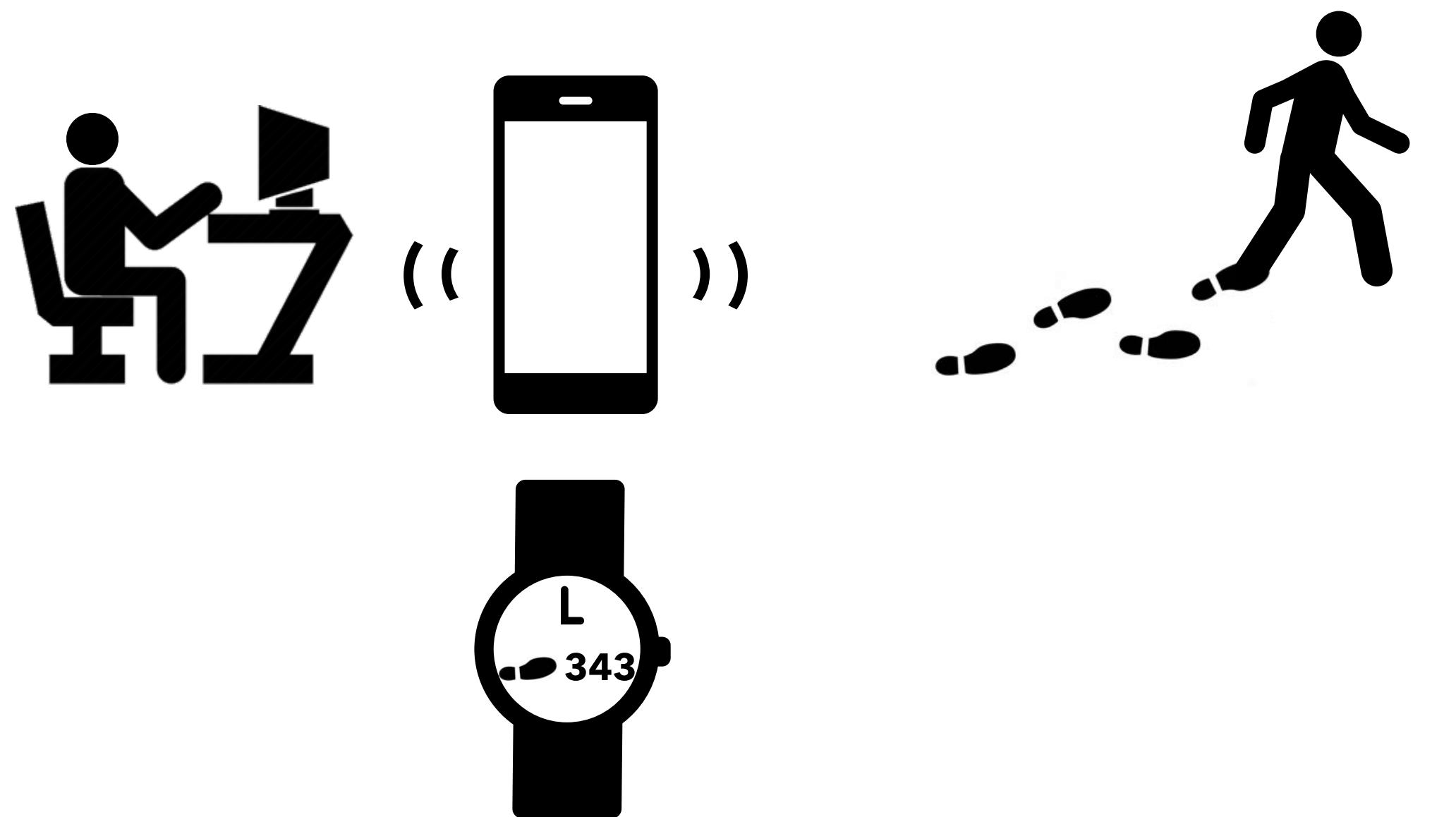


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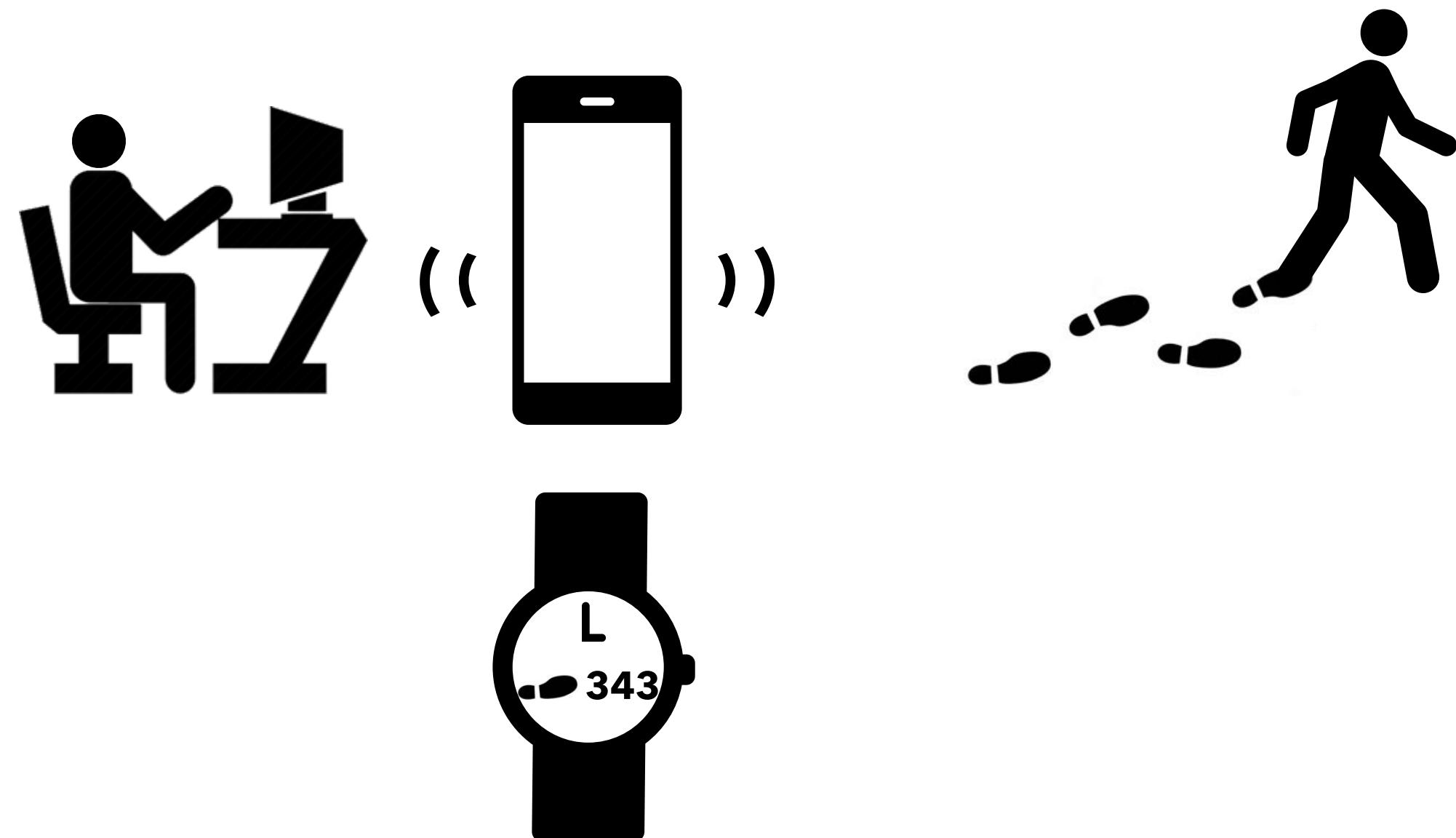
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After-study personalized inference questions

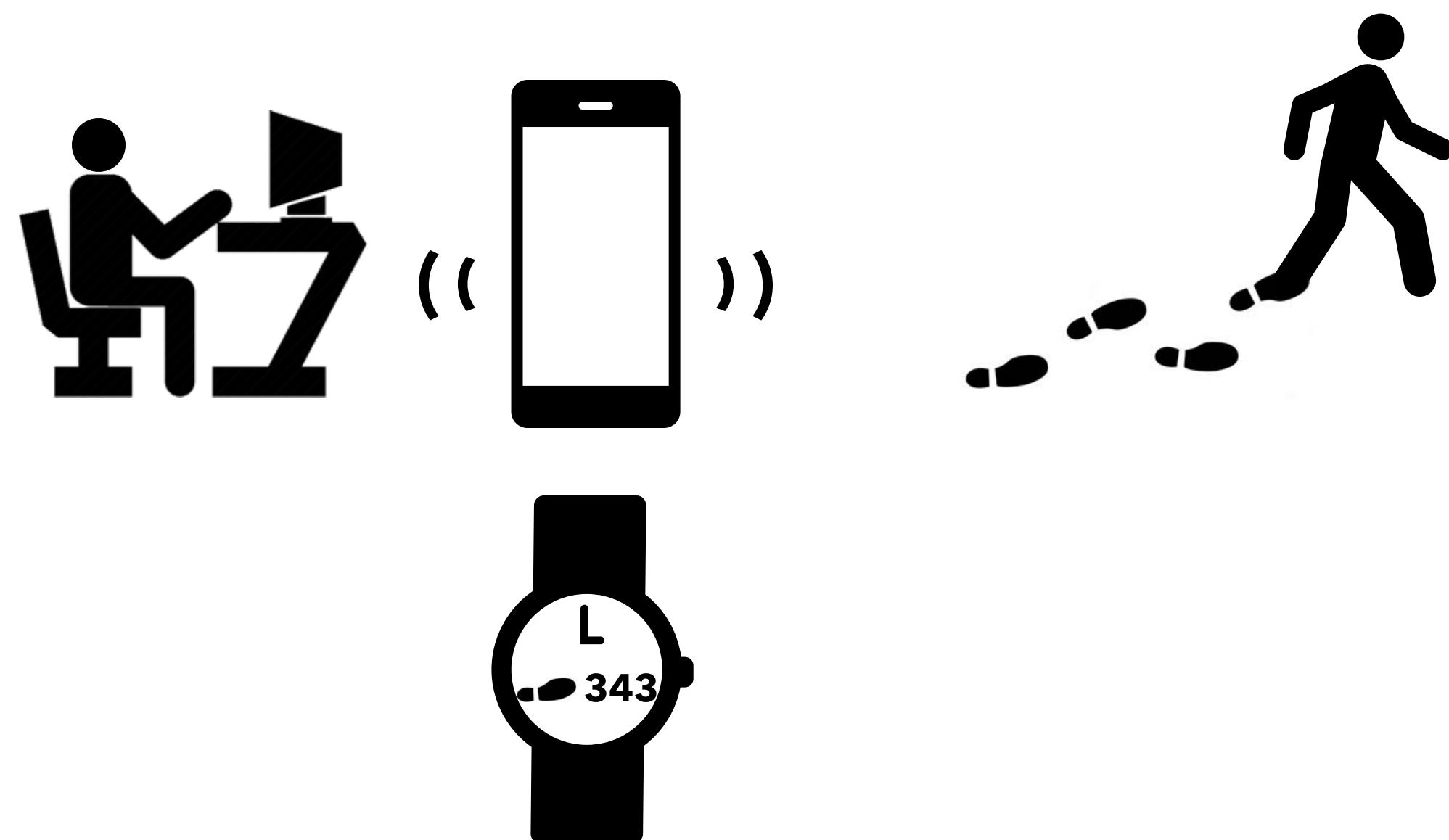
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❓ Did the app increase physical activity for a given user?



After-study personalized inference questions

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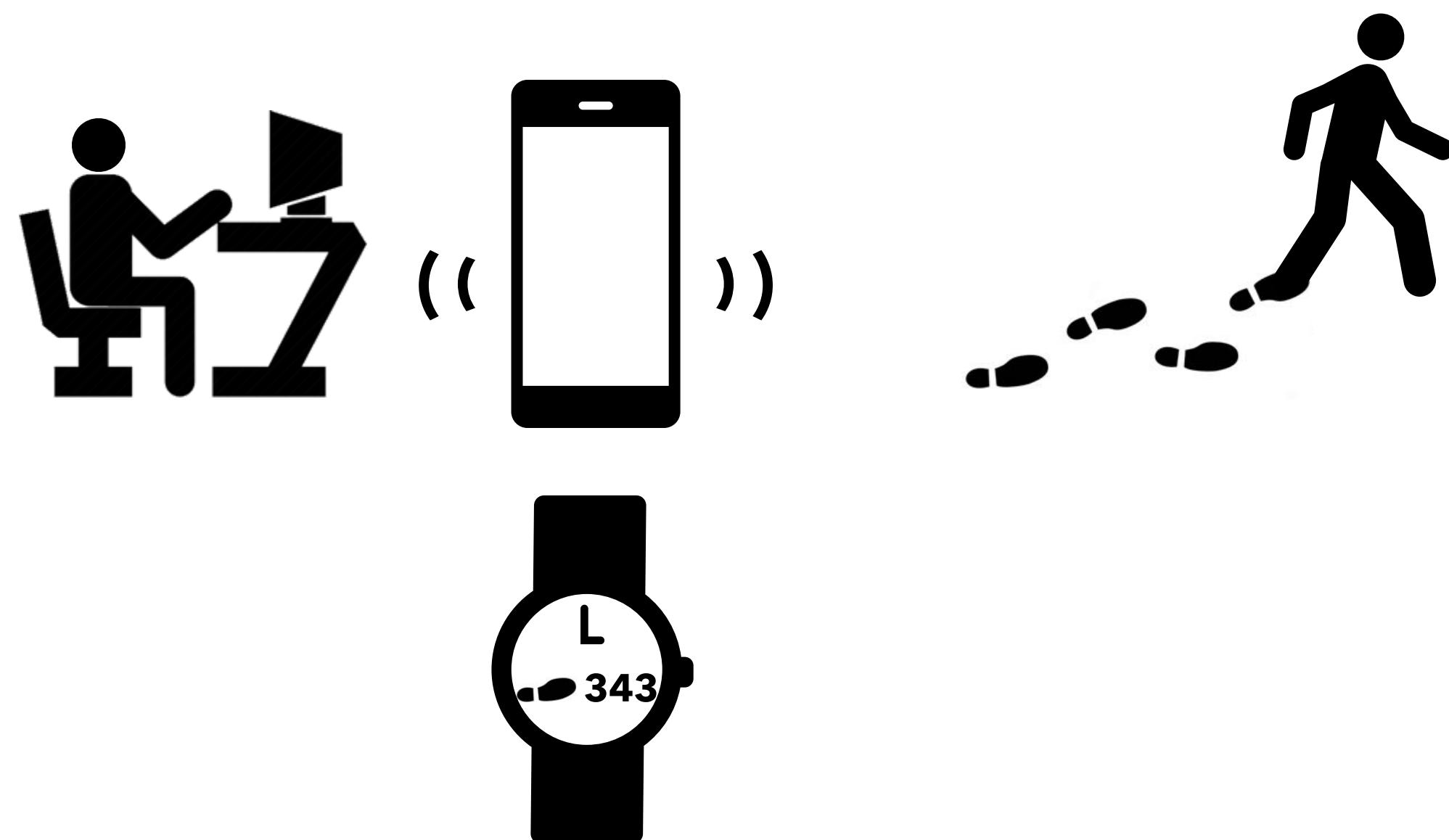


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Was sending the notification effective?

After-study personalized inference questions

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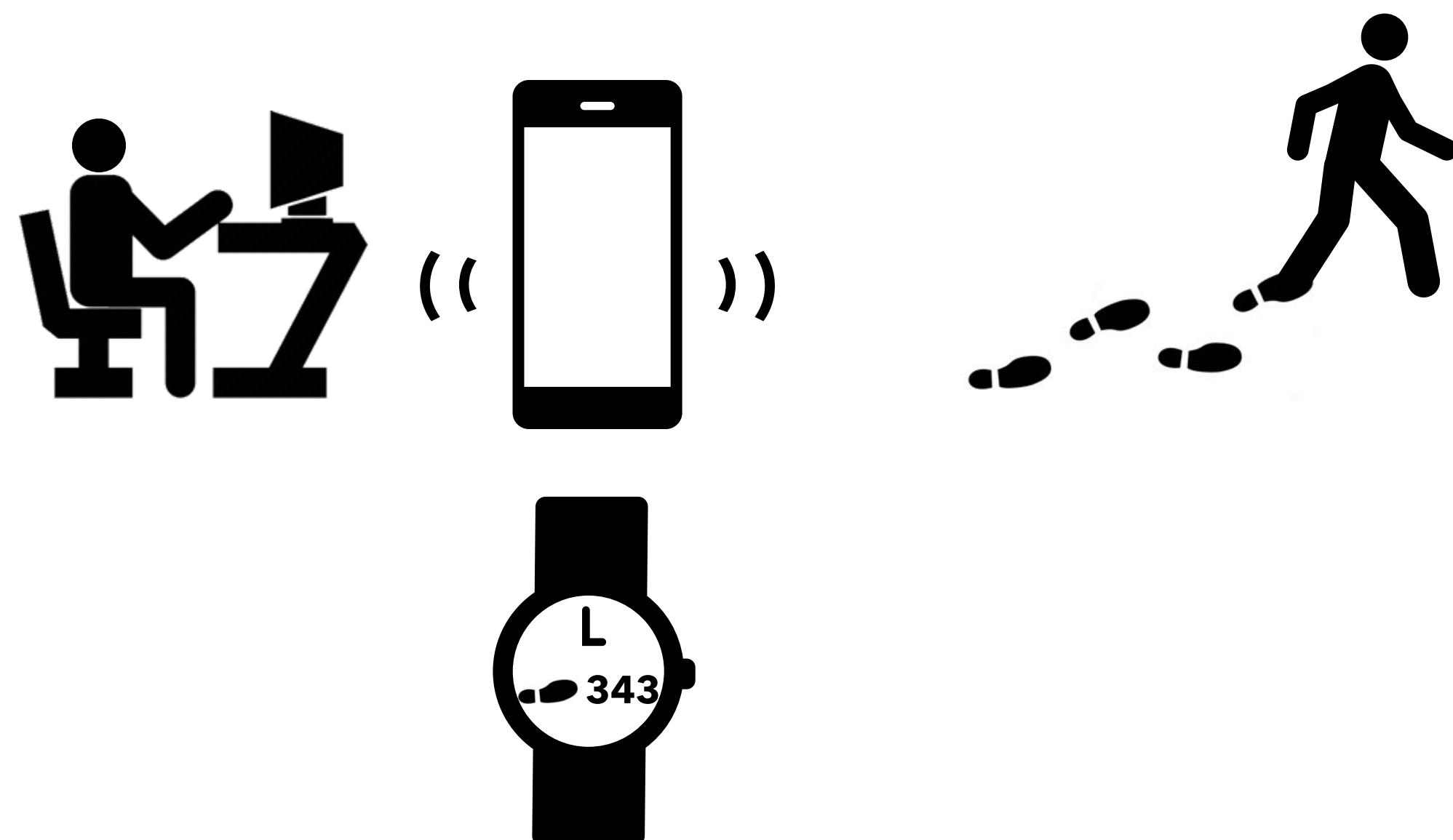
❓ Did the app increase physical activity for a given user?

Was sending the notification effective?

Was the bandit algorithm effective?

After-study personalized inference questions

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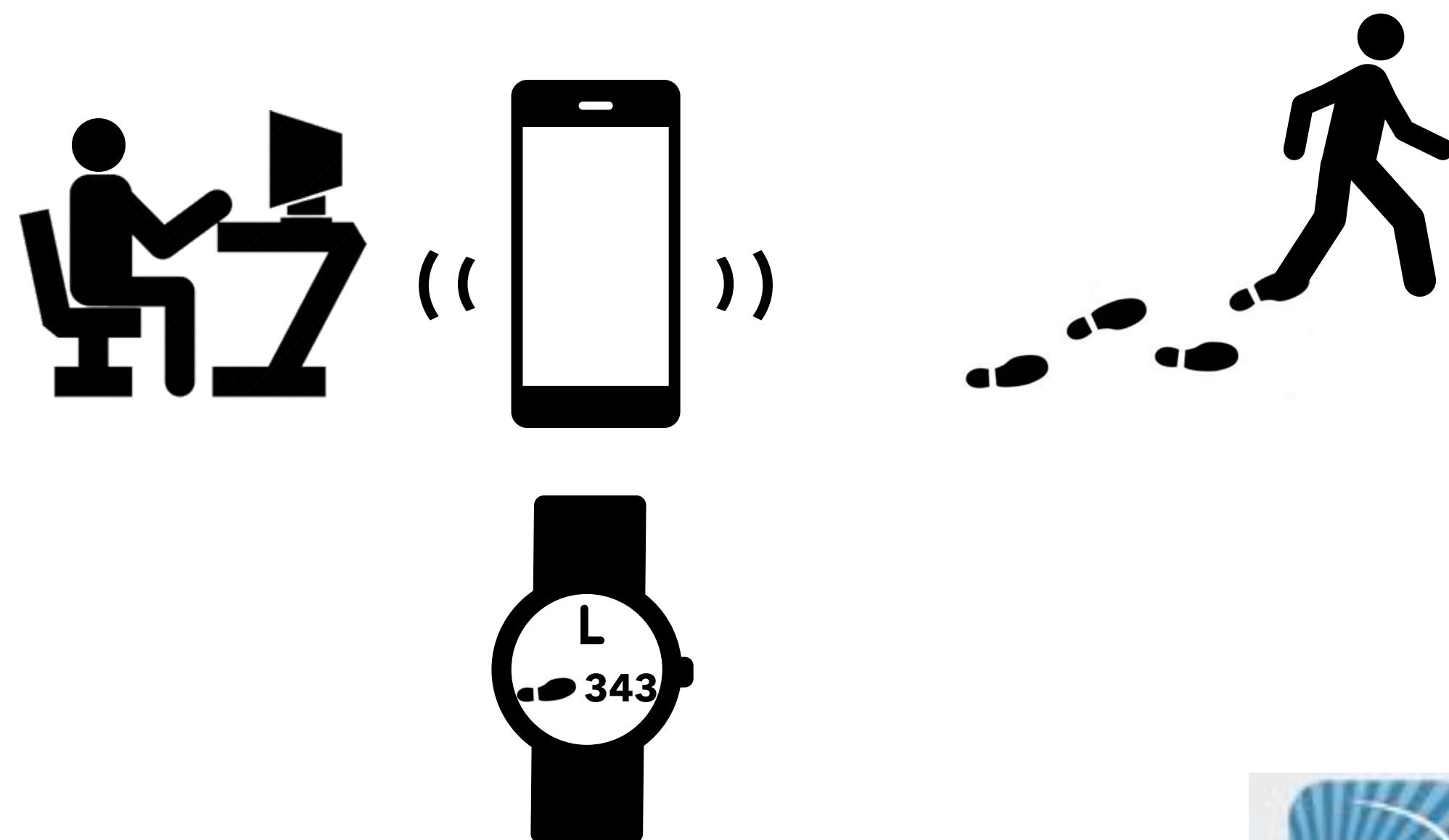
Was sending the notification effective?

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➡️ **Challenges:** Lack of mechanistic models, adaptively collected data, expensive data collection

After-study personalized inference questions

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VA Mobile Apps

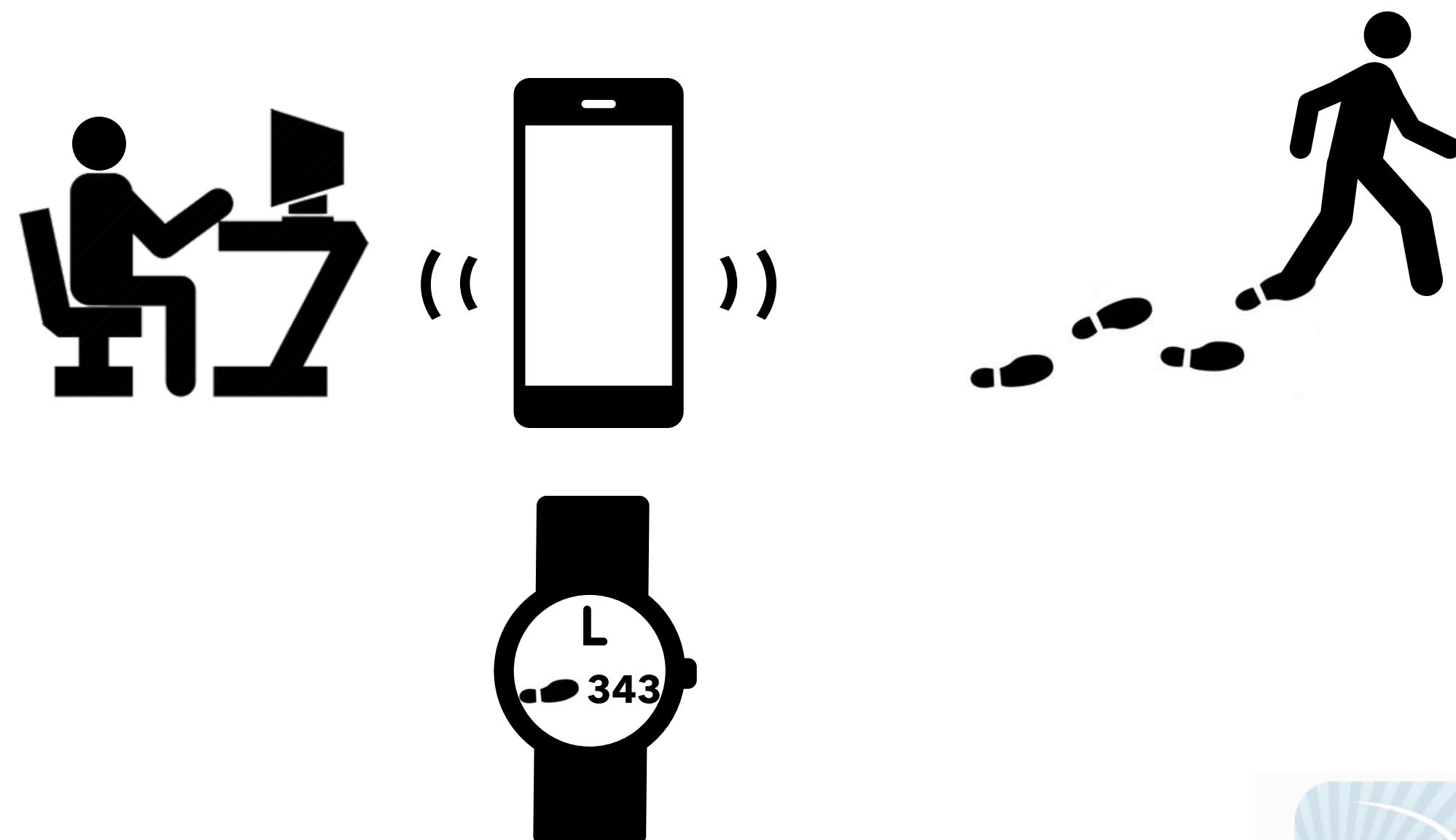
Part 1 overview: Sample-efficient personalized inference in sequential experiments



How to assign personalized digital treatments to help you?

Did the app increase physical activity for a given user?

This talk



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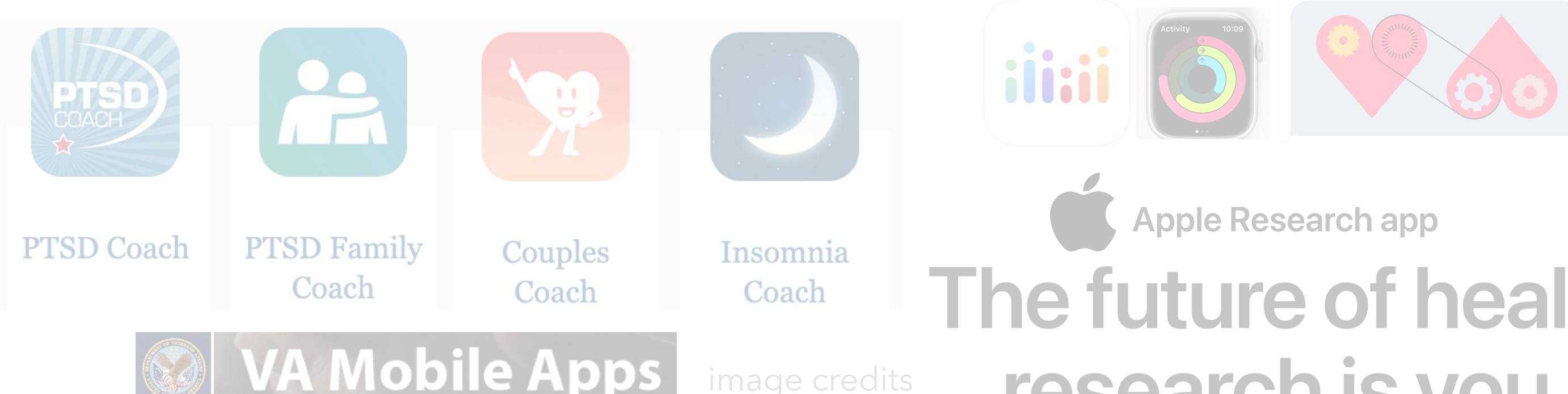


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The future of health research is you.

Problem set-up



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For user $i \in [N]$ at time $t \in [T]$

$A_{i,t}$: treatment $\in \{0,1\}$ (send a notification
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Problem set-up



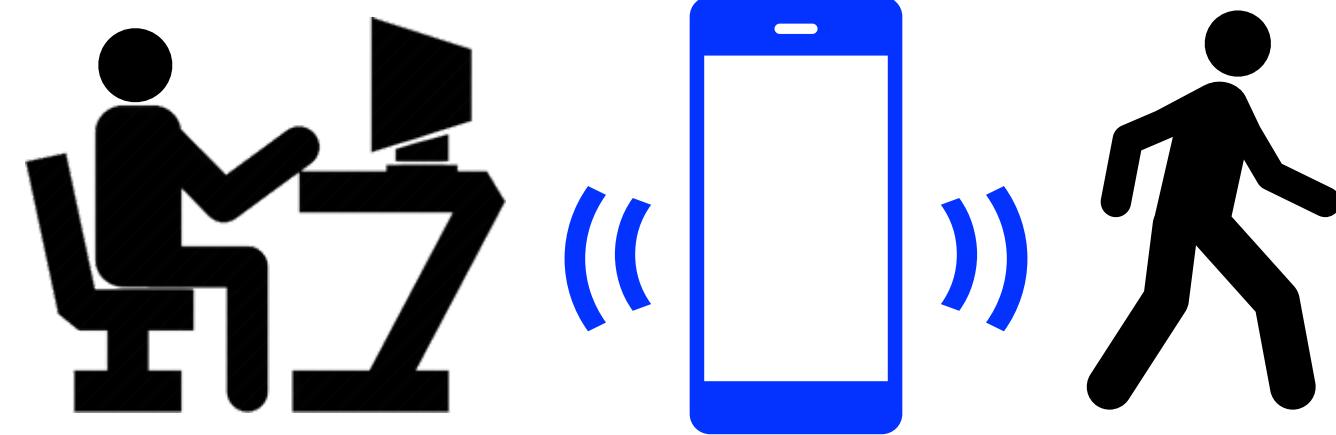
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e.g., ϵ -greedy, Thompson sampling, softmax, multiplicative weights, pooled variants,...

Sequentially adaptive policy that **can pool** observed data **across users** to speed up learning

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[Neyman-Rubin framework

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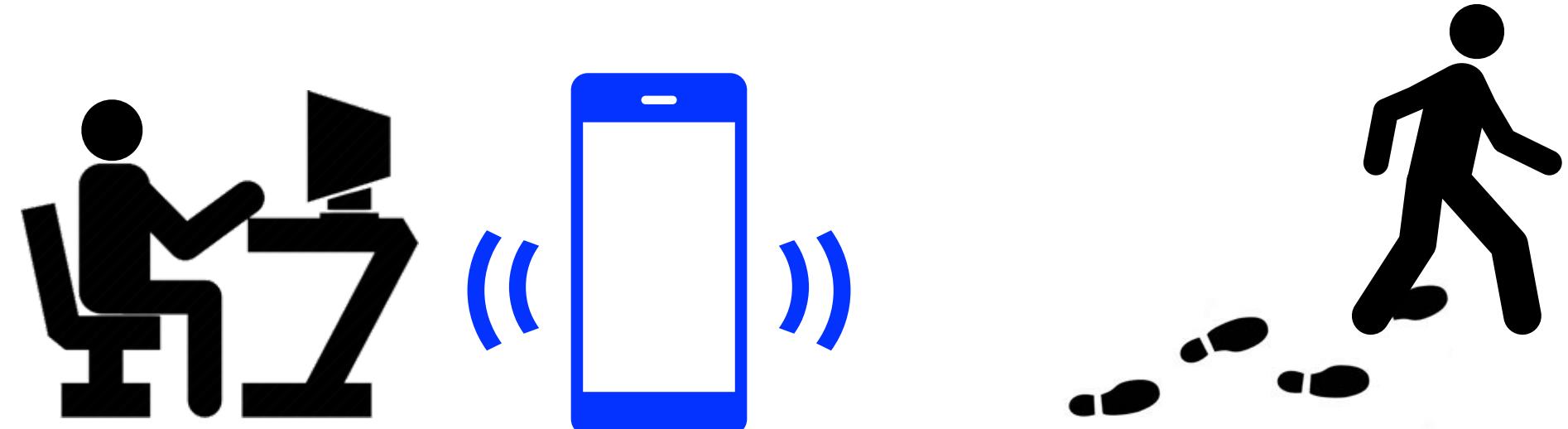
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outcome observed:

$$Y_{i,t} = \theta_{i,t}^{(A_{i,t})} + \text{noise}_{i,t}$$

[Neyman-Rubin framework
+ SUTVA]

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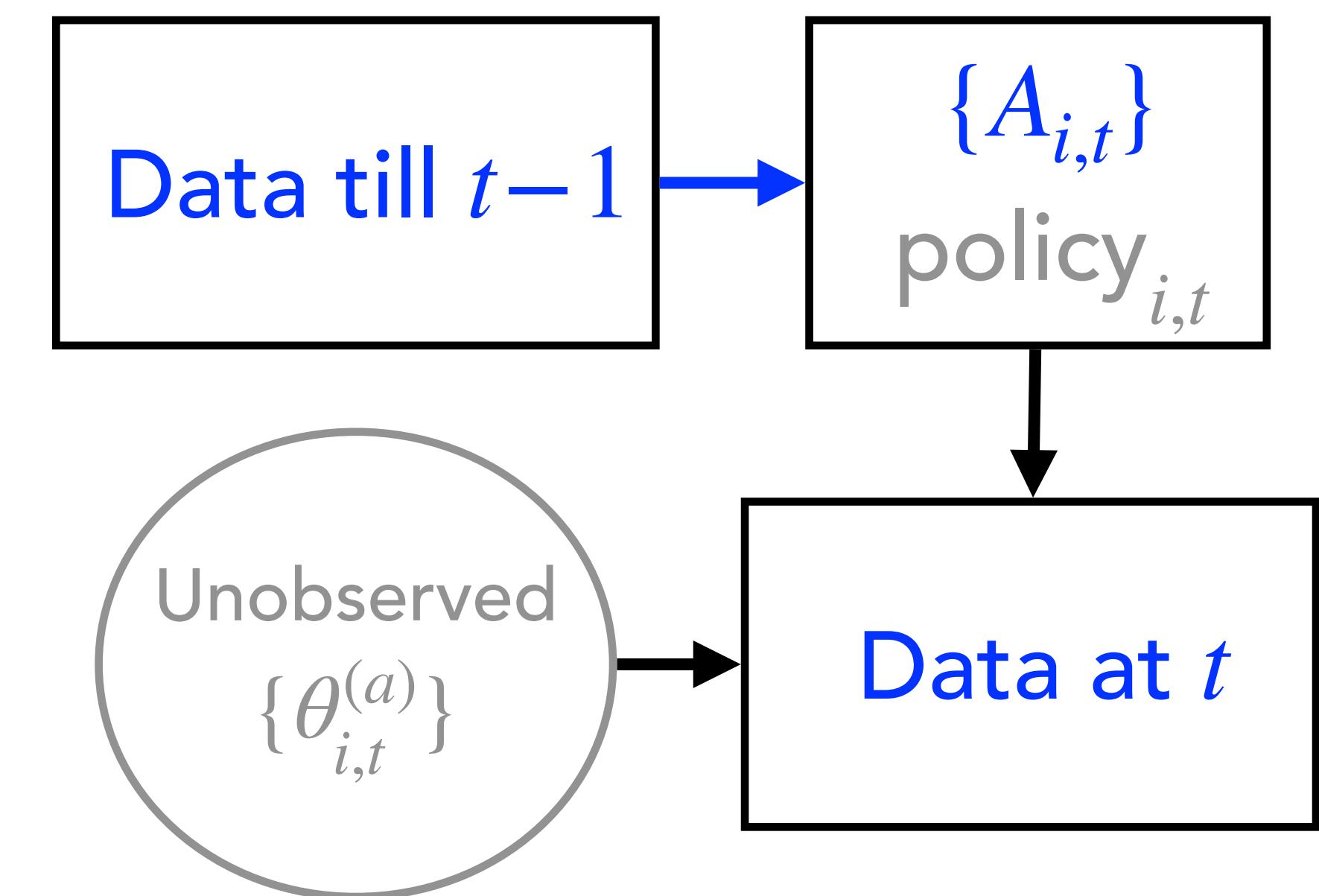
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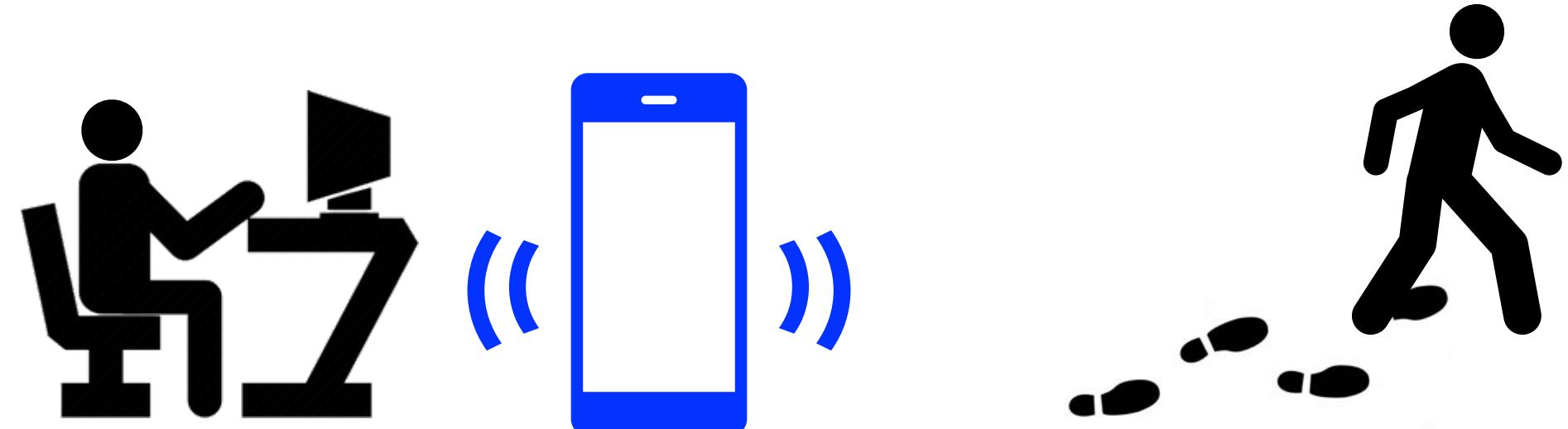
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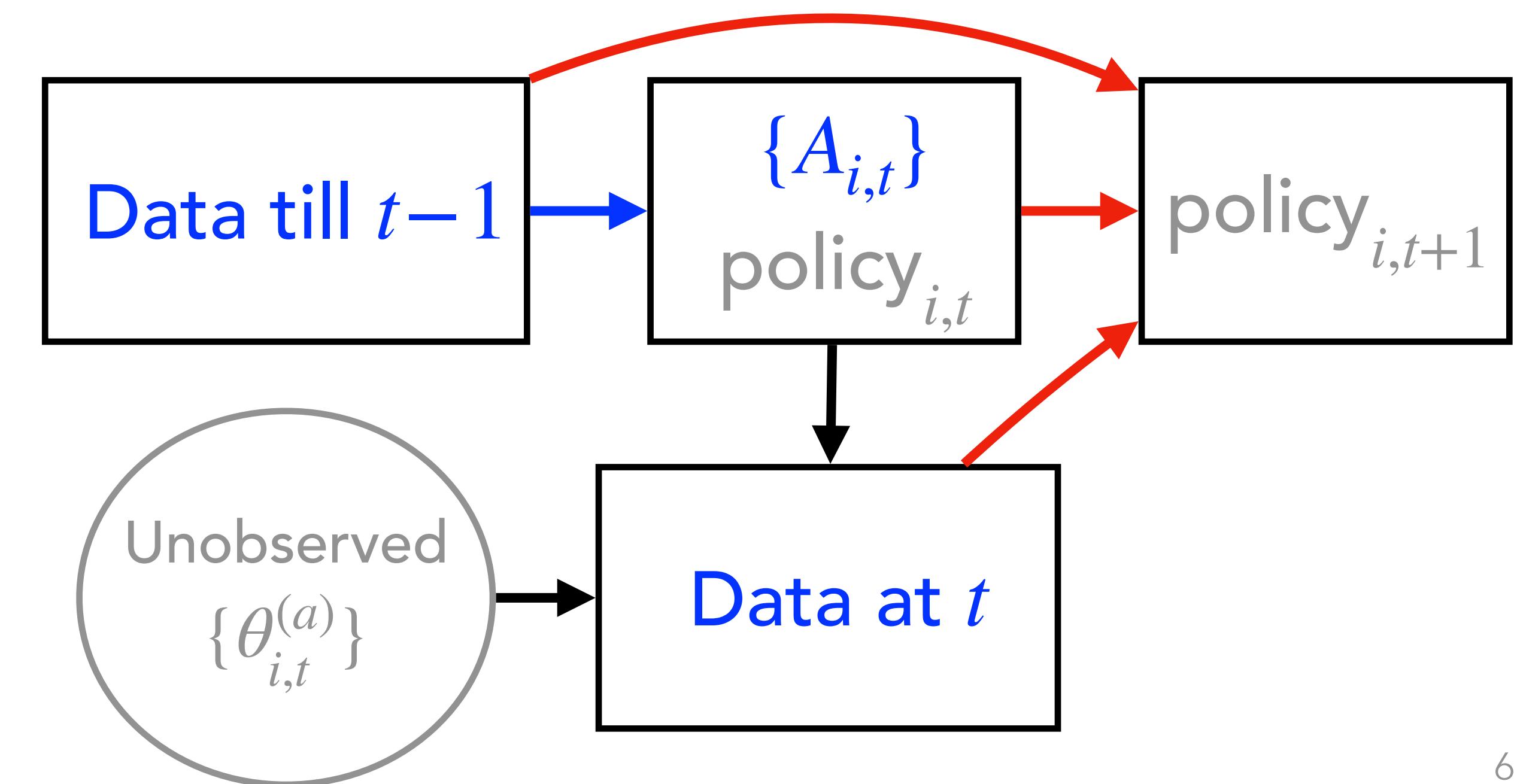
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Sequentially adaptive policy that can pool observed data **across users** to speed up learning

Estimate counterfactual means $\{\theta_{i,t}^{(a)}\}$ for $a \in \{0,1\}$, **all** N users & T times

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Estimate counterfactual means $\{\theta_{i,t}^{(a)}\}$ for $a \in \{0,1\}$, **all** N users & T times

- Enable generic after-study analyses and assist next study design
- E.g., how effective was the notification for user i at time t ($\theta_{i,t}^{(1)} - \theta_{i,t}^{(0)}$)?

Estimate counterfactual means $\{\theta_{i,t}^{(a)}\}$ for $a \in \{0,1\}$, all N users & T times

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Challenges:

- More unknowns than (noisy) observations

An impossible task without structural assumptions...

Estimate counterfactual means $\{\theta_{i,t}^{(a)}\}$ for $a \in \{0,1\}$, all N users & T times

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Hope:

- ★ N iid users
- ★ T (dependent) observations per user
- ★ If users are not all too different & multiple observations can help find similarities

A possible task with some structural assumptions...

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Challenges:

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Prior work:

- **Average treatment effect**

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Prior work:

- Average treatment effect
 - IID users & deterministic rules/policies

[... Robins '94, '97, '00, '08, Murphy '03, '05, Hernan+ '06, Moodie+ '07,

Estimate counterfactual means $\{\theta_{i,t}^{(a)}\}$ for $a \in \{0,1\}$, all N users & T times

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Prior work:

- **Average treatment effect**
 - IID users & deterministic rules/policies
 - IID users at each time with stochastic policies

[... Robins '94, '97, '00, '08, Murphy '03, '05, Hernan+ '06, Moodie+ '07, ... Deshpande+ '18, Hadad+ '21, Bibaut+ '21, Khamaru+ '21, Zhang+ '21,

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 - IID users at each time with stochastic policies
 - IID user trajectories (per user policy, no pooling)

[... Robins '94, '97, '00, '08, Murphy '03, '05, Hernan+ '06, Moodie+ '07, ... Deshpande+ '18, Hadad+ '21, Bibaut+ '21, Khamaru+ '21, Zhang+ '21,

Estimate counterfactual means $\{\theta_{i,t}^{(a)}\}$ for $a \in \{0,1\}$, all N users & T times

Challenges:

- More unknowns than (noisy) observations
- No parametric model available
- Intricate dependencies due to
 - Heterogeneity across users and time
 - Sequentially adaptive policy
 - Pooling for policy design

An impossible task without structural assumptions...

Prior work:

- **Average treatment effect**
 - IID users & deterministic rules/policies
 - IID users at each time with stochastic policies
 - IID user trajectories (per user policy, no pooling)
- **Observational studies** (once treated forever treated; synthetic control, causal panel data)

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Structural assumption: Non-parametric factor model

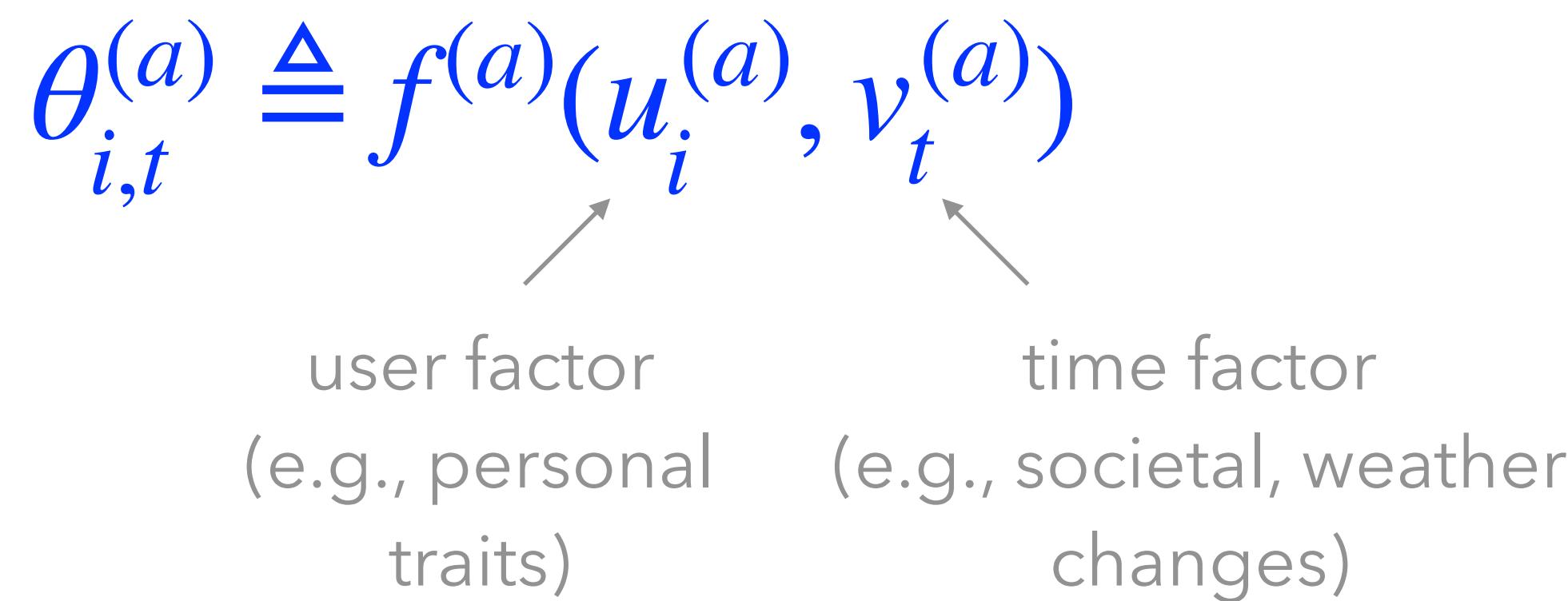
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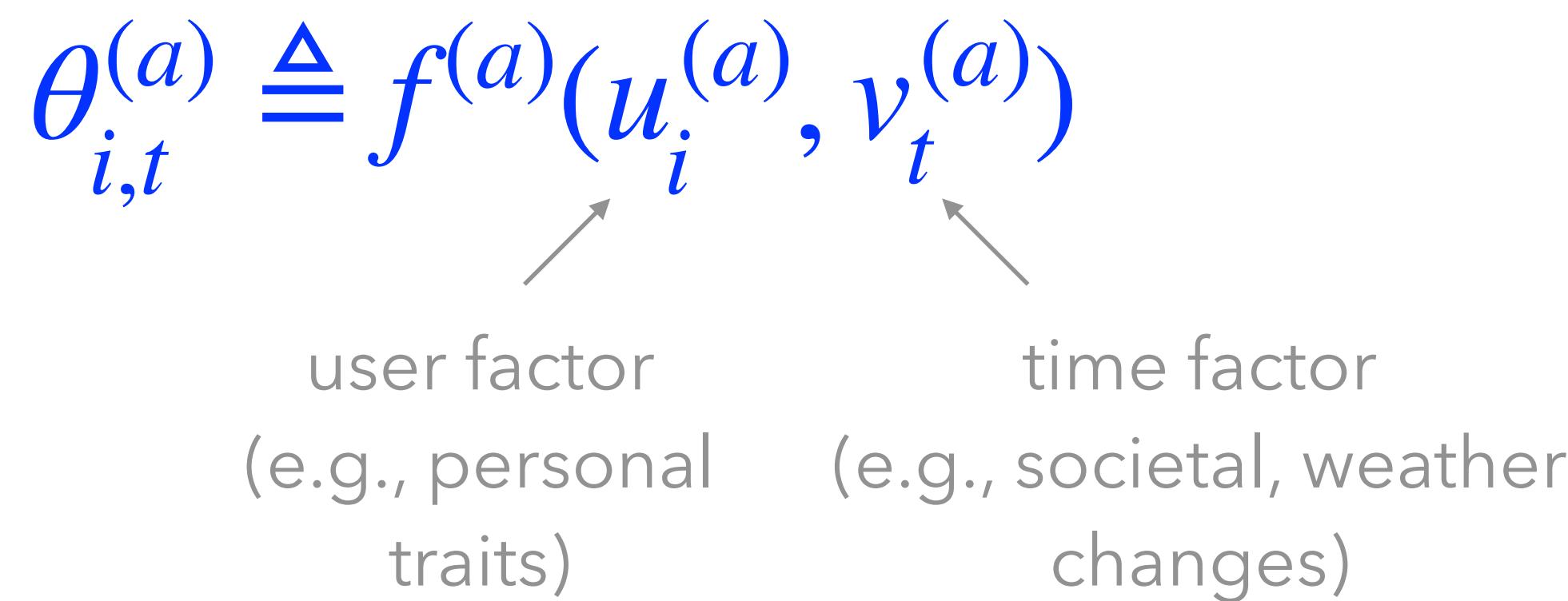
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user factor time factor
(e.g., personal traits) (e.g., societal, weather changes)



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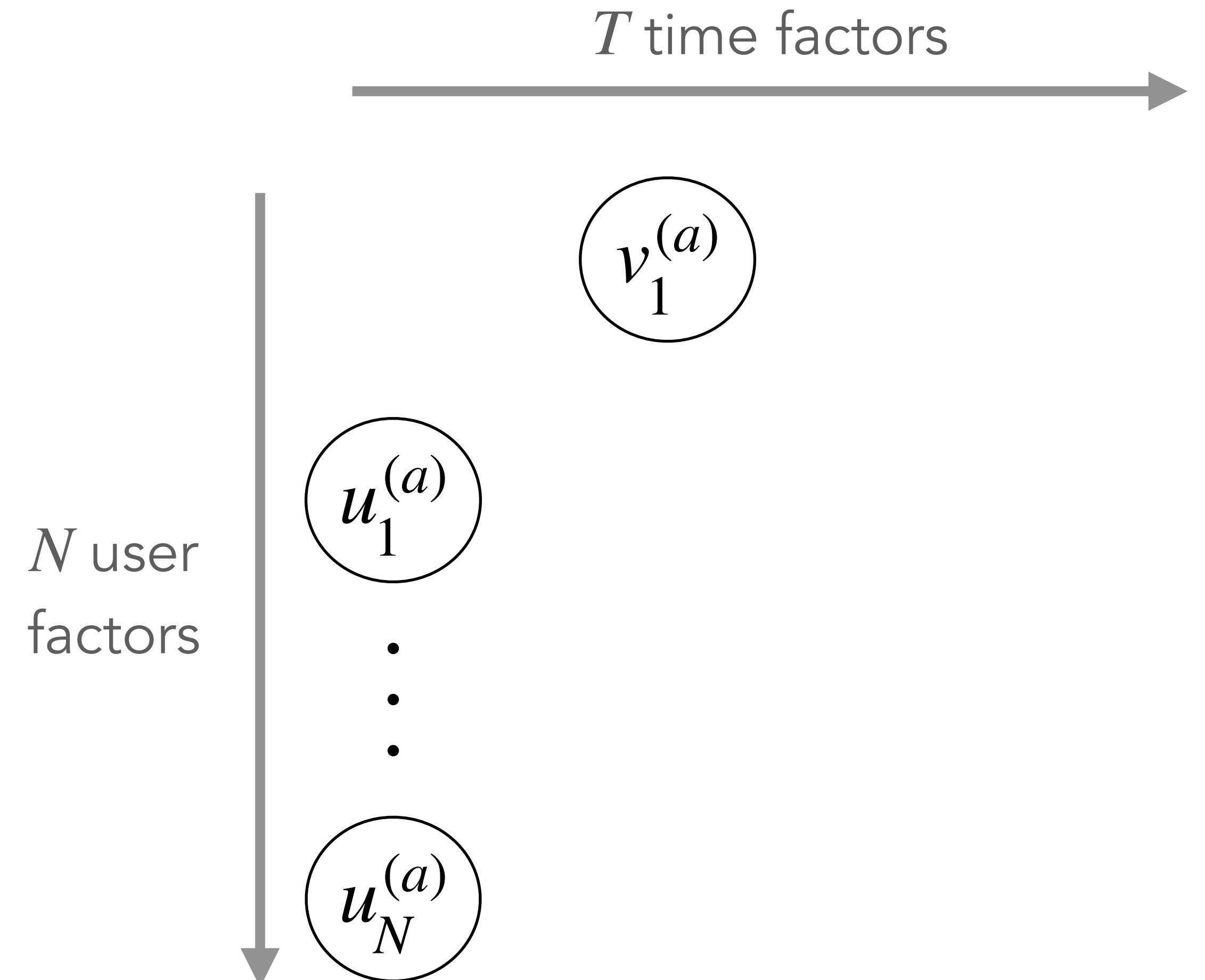
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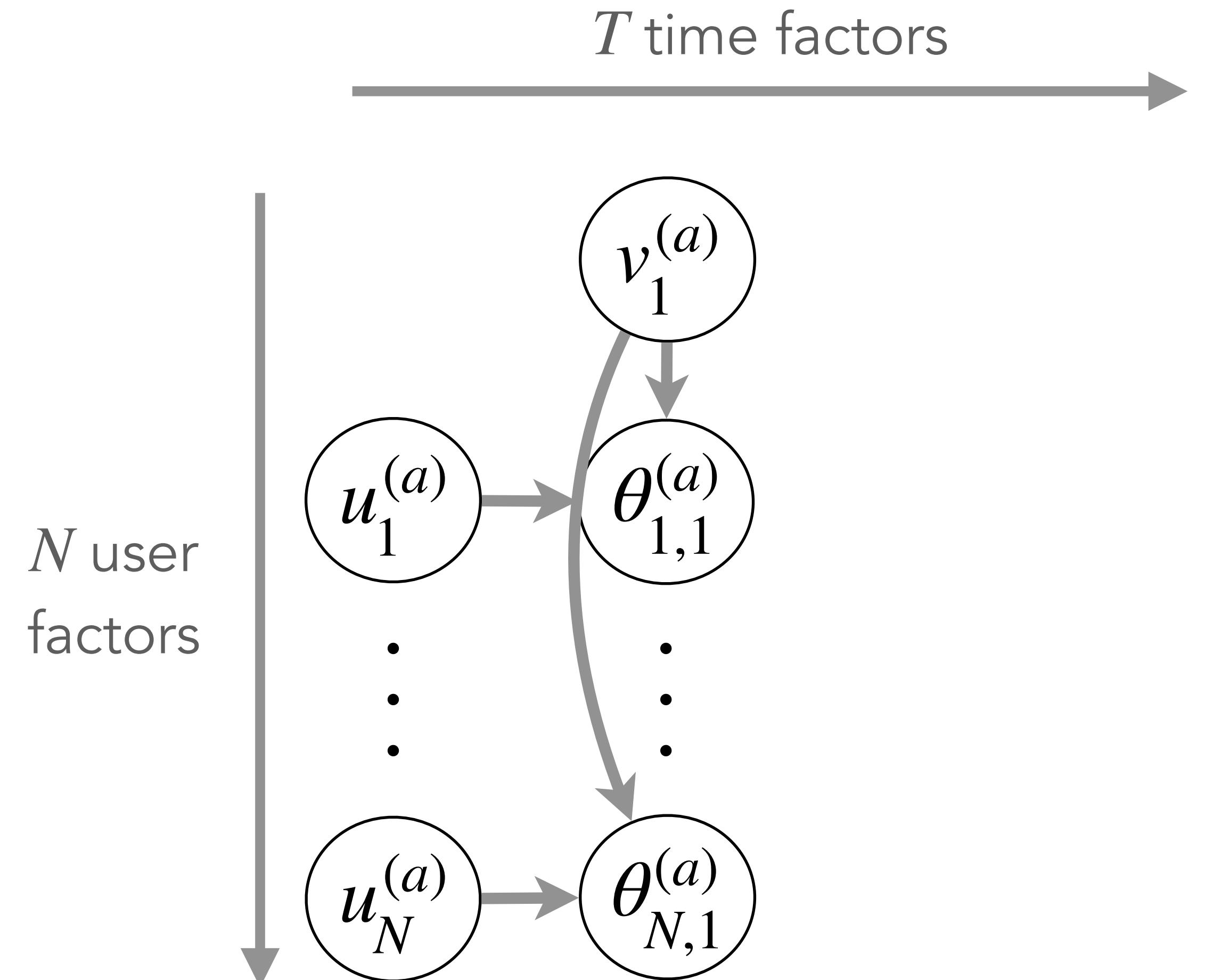
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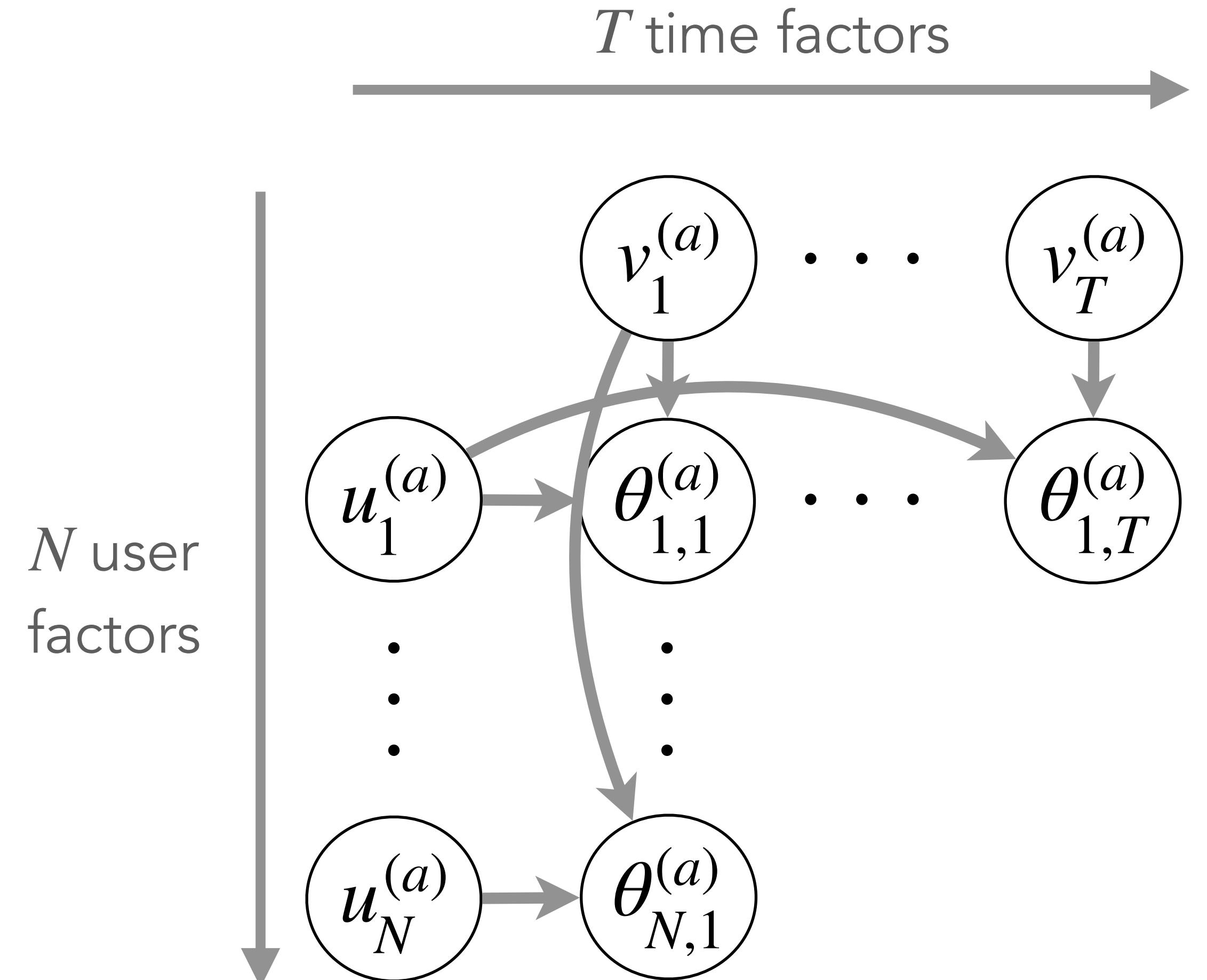
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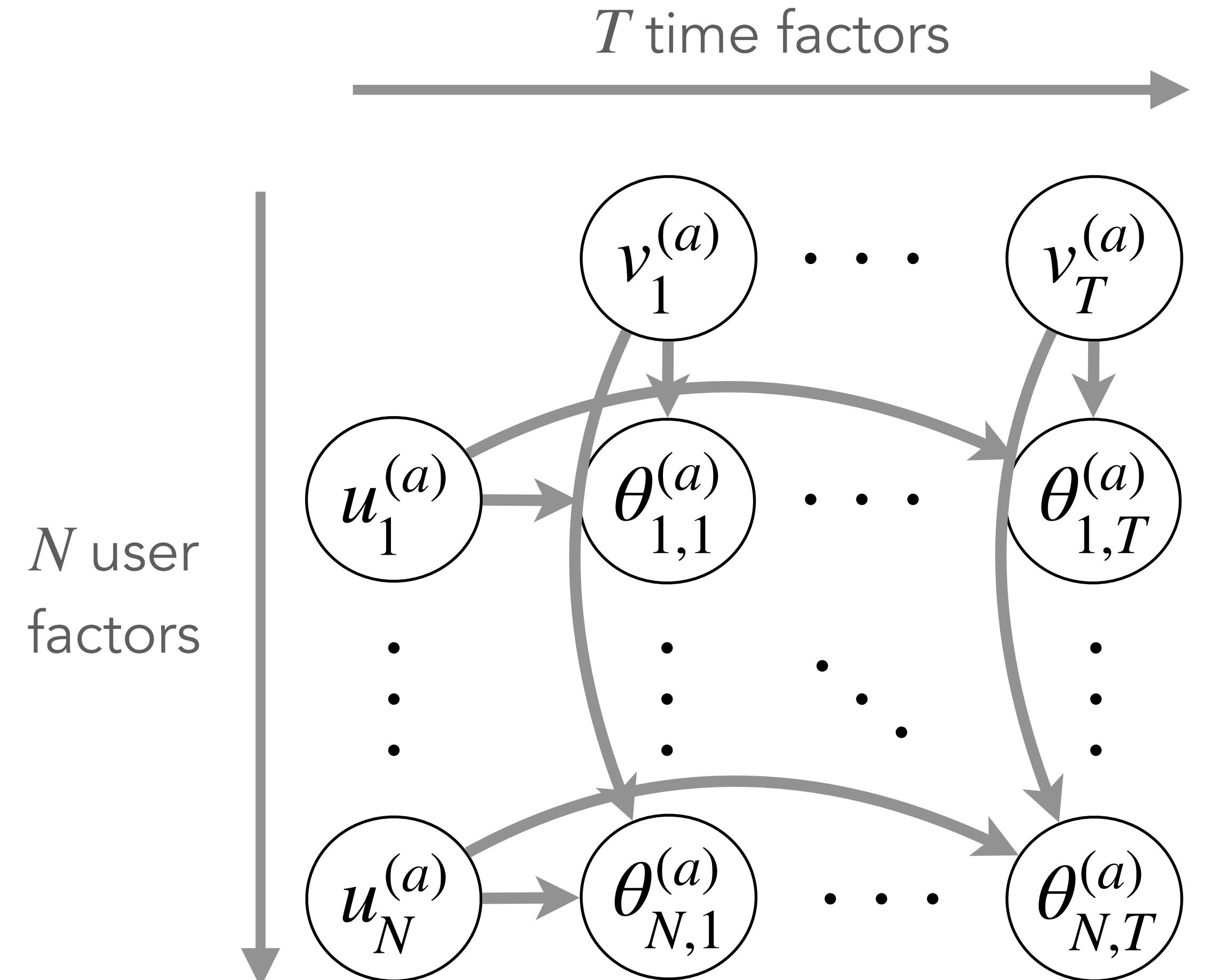
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User nearest neighbors estimator for $\theta_{i,t}^{(a)}$

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$$\rho_{i,j}^{(a)} = \frac{\sum_{t'=1}^T (Y_{i,t'} - Y_{j,t'})^2 \cdot \mathbf{1}(A_{i,t'} = A_{j,t'} = a)}{\sum_{t'=1}^T \mathbf{1}(A_{i,t'} = A_{j,t'} = a)}$$

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Squared distance between outcomes
averaged over **all times when i and j are both treated with a**

2. Average outcome across **user neighbors treated with a at time t**

$$\hat{\theta}_{i,t,\text{user-NN}}^{(a)} = \frac{\sum_{j=1}^N Y_{j,t} \cdot \mathbf{1}(\rho_{i,j}^{(a)} \leq \eta, A_{j,t} = a)}{\sum_{j=1}^N \mathbf{1}(\rho_{i,j}^{(a)} \leq \eta, A_{j,t} = a)}$$

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$$|\hat{\theta}_{i,t,\text{user-NN}}^{(a)} - \theta_{i,t}^{(a)}| \lesssim \frac{1}{T^{1/4}} + \frac{1}{(N/M)^{1/2}}$$

User factor distribution



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User-NN guarantees: Advantages

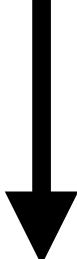
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- Asymptotic **confidence intervals** as $N, T \rightarrow \infty$:

$$\hat{\theta}_{i,t,\text{user-NN}}^{(a)} \pm \frac{1.96 \hat{\sigma}}{\sqrt{\#\text{neighbors}_{i,t,a}}}$$

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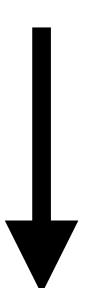
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Challenges tackled: First guarantee

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Challenges tackled: First guarantee for user-time-level counterfactuals

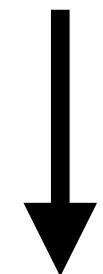
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Can we improve the slow rate in T?

Yes, we can!

A near-quadratic improvement over user-NN

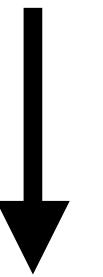
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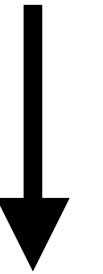
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*for Lipschitz non-linearity with Lipschitz gradients & non-adaptive policies

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$$\Rightarrow \text{??} = \hat{u}_i v_t + u_i \hat{v}_t - \hat{u}_i \hat{v}_t$$

DR-NN error \approx **user-NN error** \times **time-NN error**

\lesssim **min{user-NN error, time-NN error}**

This is our improved nearest neighbors estimator!

$$u_i v_t - \text{??} = (u_i - \hat{u}_i) \times (v_t - \hat{v}_t)$$

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DR-NN error \approx **user-NN error** \times **time-NN error**

\lesssim **min{user-NN error, time-NN error}**

Doubly robust to heterogeneity in user factors & time factors

Double robustness, double machine learning...

[... Cassel+ '77, Robinson '88, Särndal+ '89, Robins+ '94, '95, '08, '09, Newey+ '94, '18, Bickel+ '98, van der Laan+ '03, Lunceford+ '04, Davidian+ '05, Li+ '11, Jiang+ '15, Chernozhukov+ '18, Hirshberg+ '18, Diaz '19, Arkhangelsky+ '21, Dorn+ '21 ...]

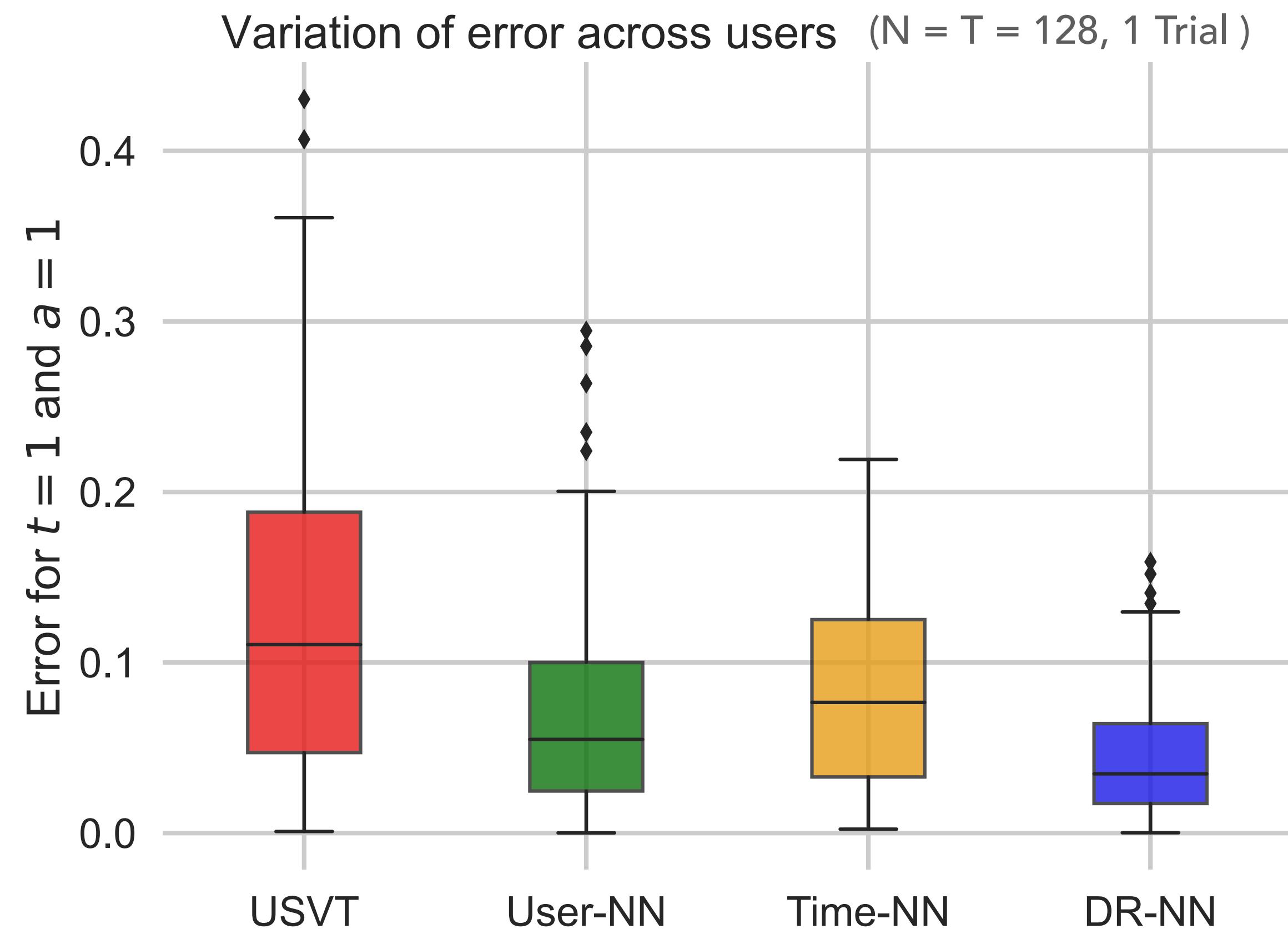
Simulation results

Simulation results

Uniform latent factors on $[-0.5,0.5]^4$, Gaussian noise, pooled ε -greedy policy ($\varepsilon = 0.5$)

Simulation results

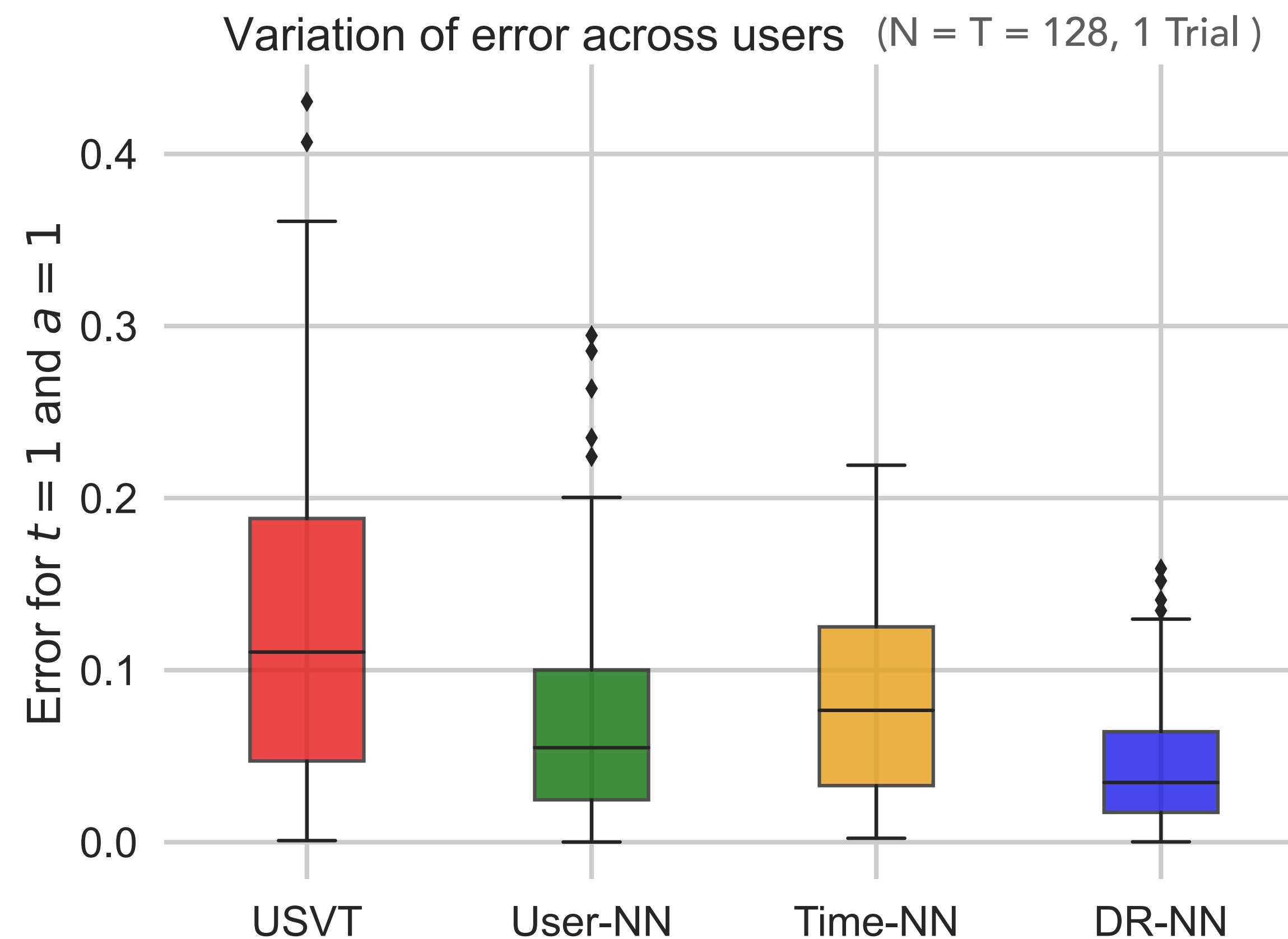
Uniform latent factors on $[-0.5,0.5]^4$, Gaussian noise, pooled ε -greedy policy ($\varepsilon = 0.5$)



A baseline
algorithm from
[Chatterjee 2014]

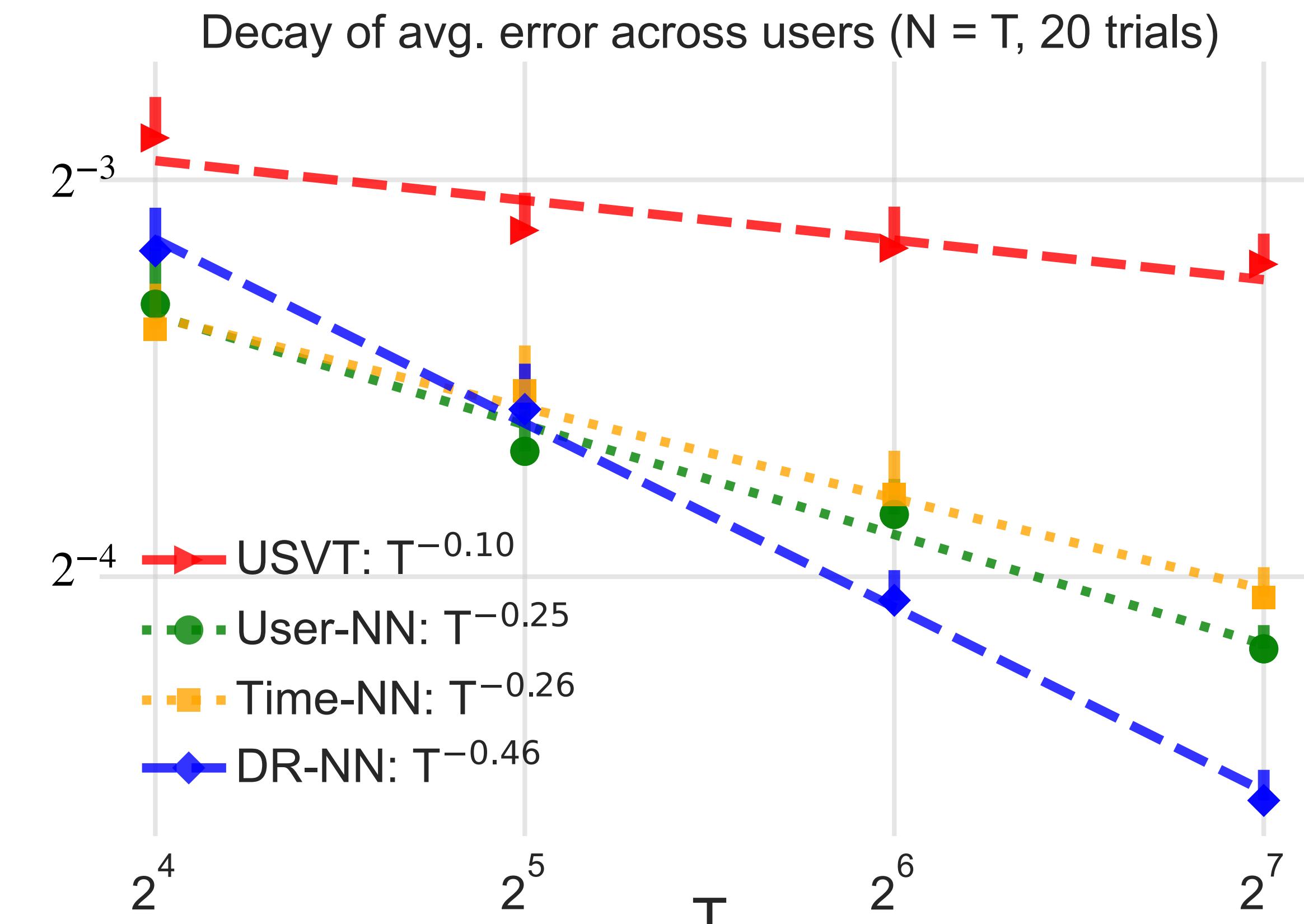
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DR-NN error ≪ min { user-NN error, time-NN error }



Personalized HeartSteps results



Personalized HeartSteps results

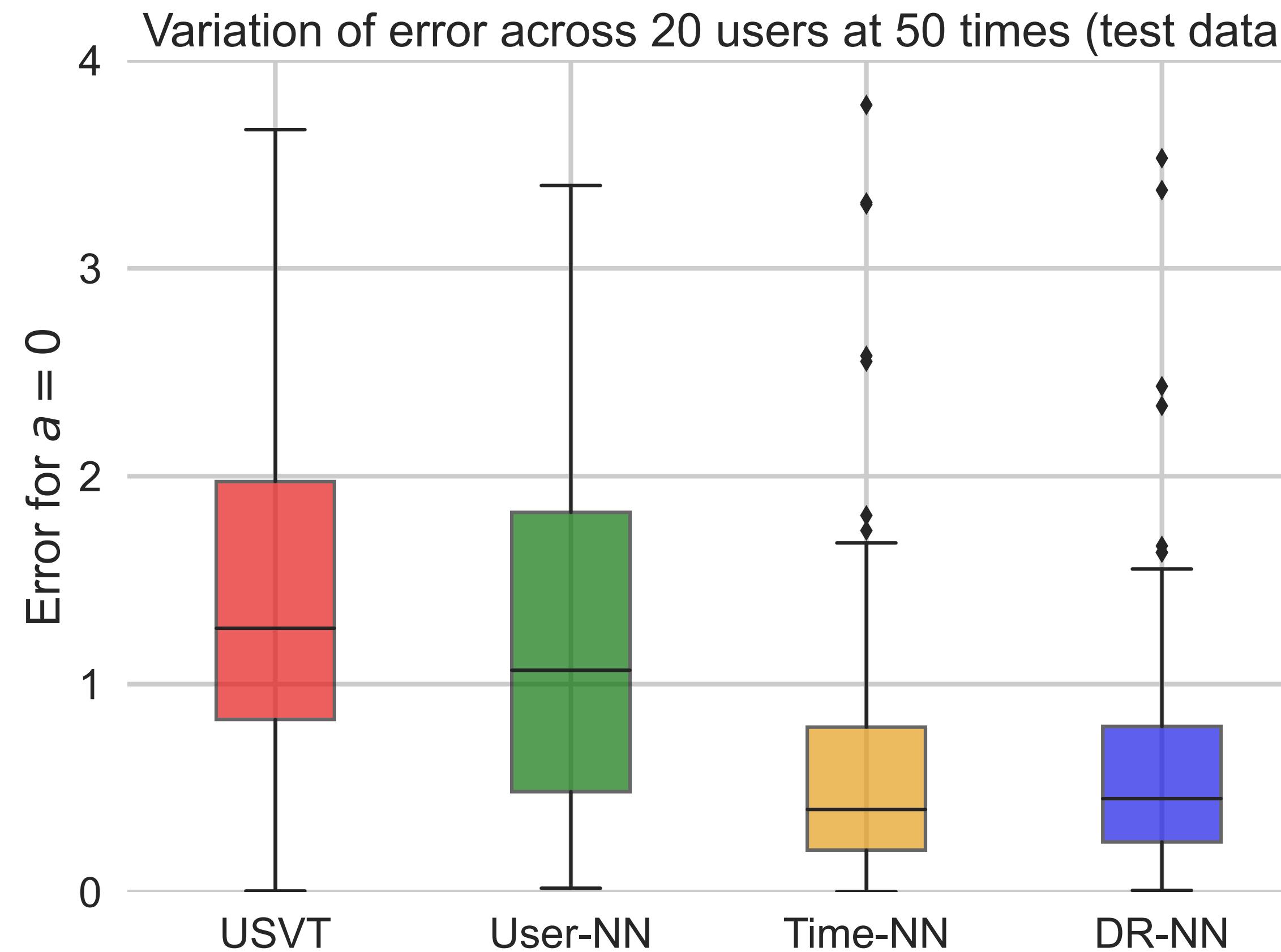


Treatments assigned with Thompson sampling independently for 91 users for 90 days, 5 times a day

Personalized HeartSteps results



Treatments assigned with Thompson sampling independently for 91 users for 90 days, 5 times a day

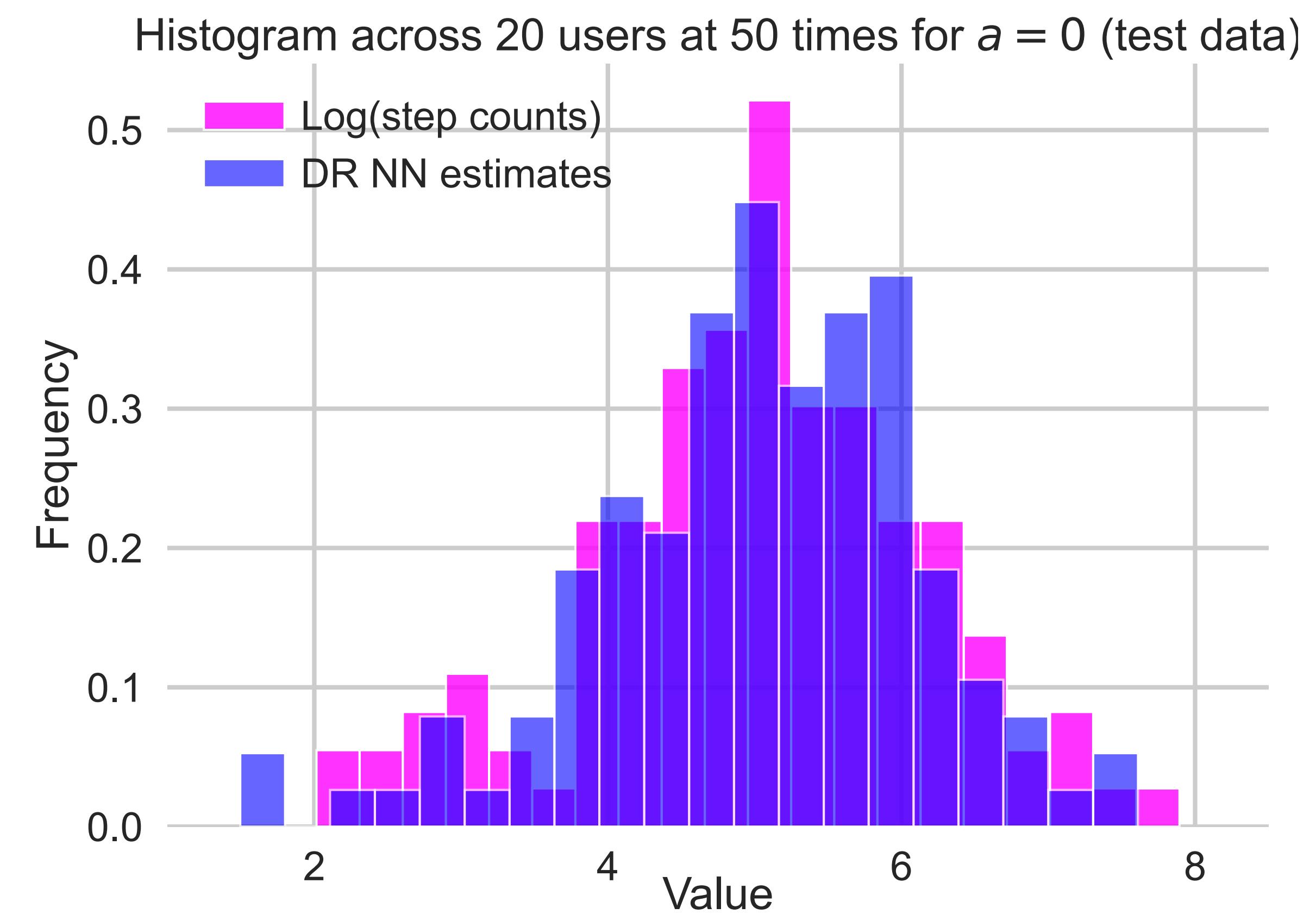
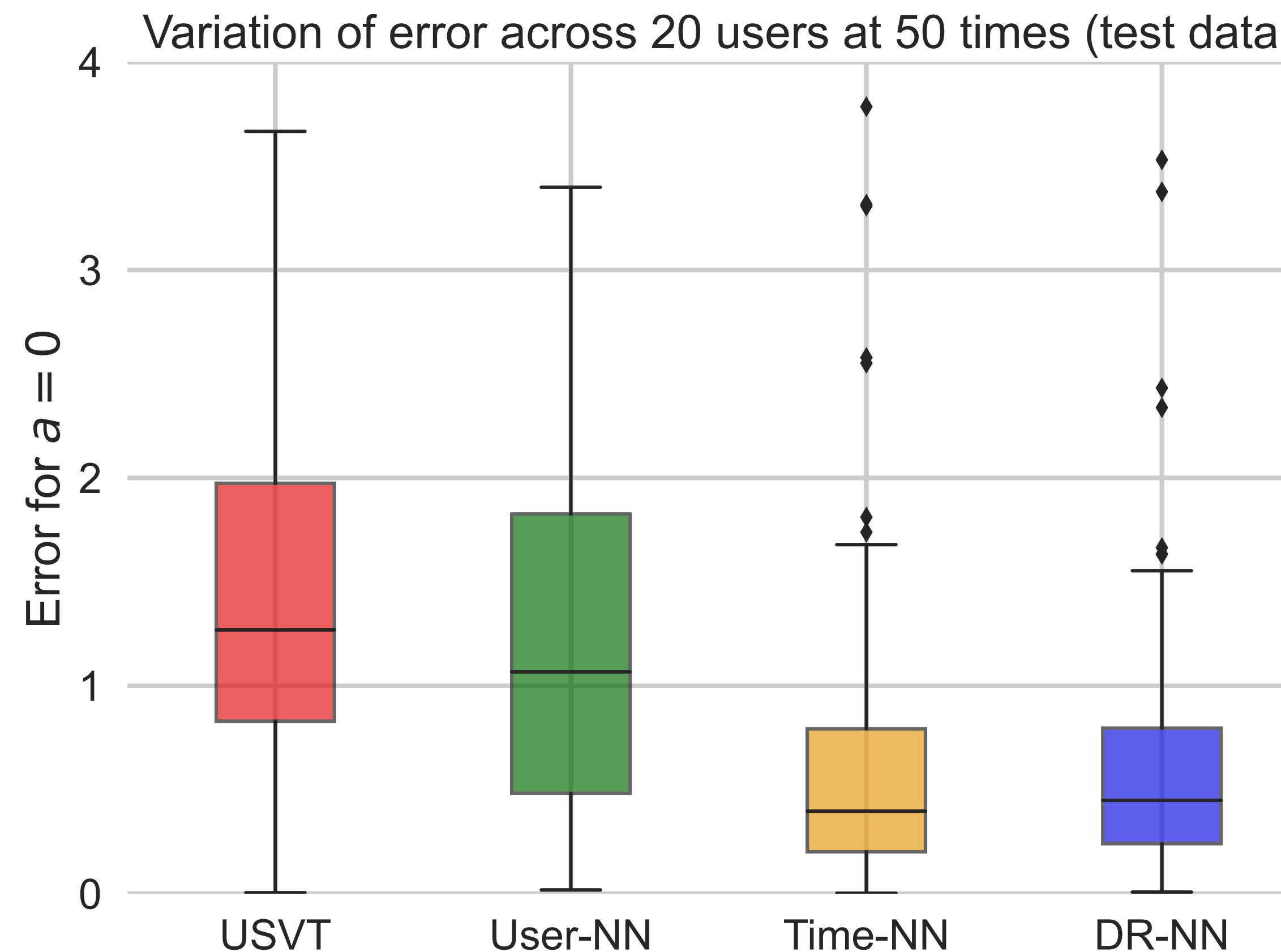


DR-NN error $\approx \min \{ \text{user-NN error, time-NN error} \}$

Personalized HeartSteps results



Treatments assigned with Thompson sampling independently for 91 users for 90 days, 5 times a day



DR-NN error $\approx \min \{ \text{user-NN error, time-NN error} \}$

Part 1 summary:

Sample-efficient inference with non-parametric factor models

Part 1 summary: Sample-efficient inference with non-parametric factor models

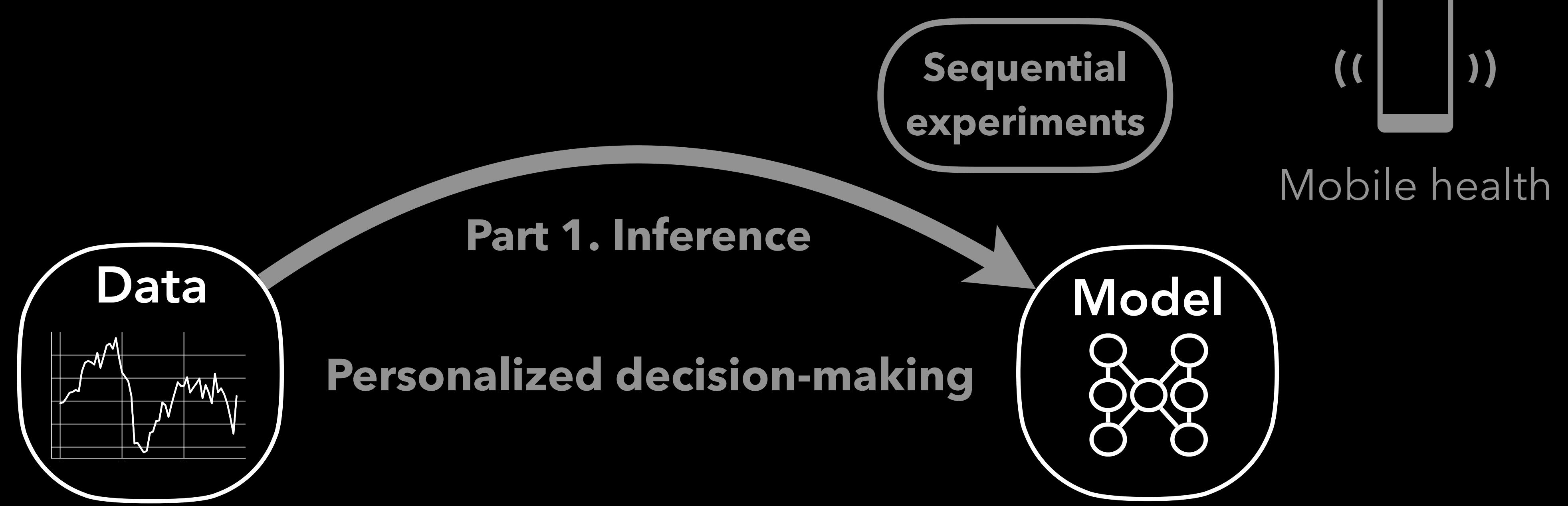
- ✓ Inference in sequential experiments: User-NN with $\tilde{O}(T^{-1/4})$ error
- ✓ Efficient estimators: Doubly robust-NN with $\tilde{O}(T^{-1/2})$ error

$$\begin{aligned}\textbf{DR-NN error} &\approx \textbf{user-NN error} \times \textbf{time-NN error} \\ &\lesssim \min\{\textbf{user-NN error}, \textbf{time-NN error}\}\end{aligned}$$

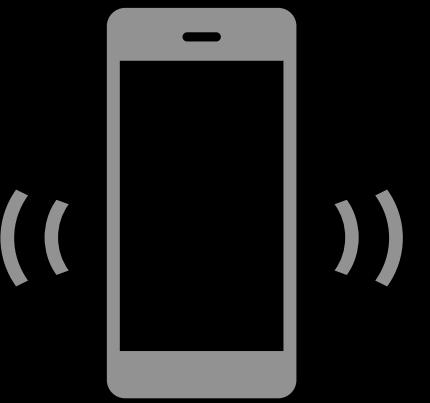


- ♦ Future: Settings with contexts and covariates

1. Use **real data** to infer decision's effect



Talk overview

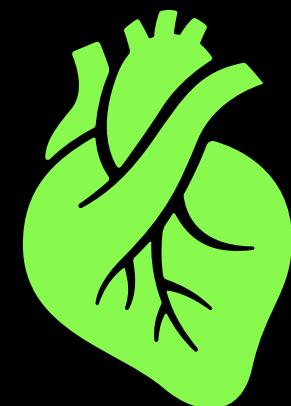


Mobile health

Sequential experiments



Data

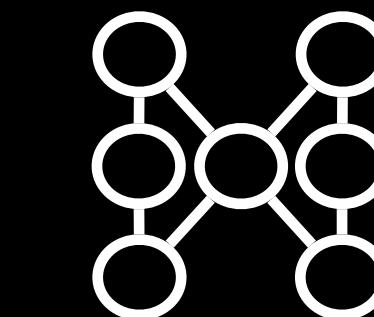


Computational
cardiology

Part 1. Inference

Personalized decision-making

Model



Part 2. Simulations

Uncertainty propagation

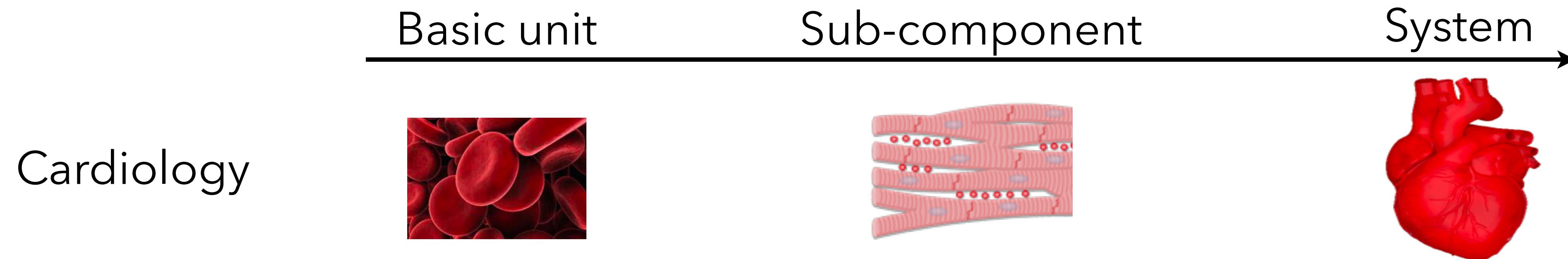
2. Use **simulated data** to predict decision's effect

Talk overview

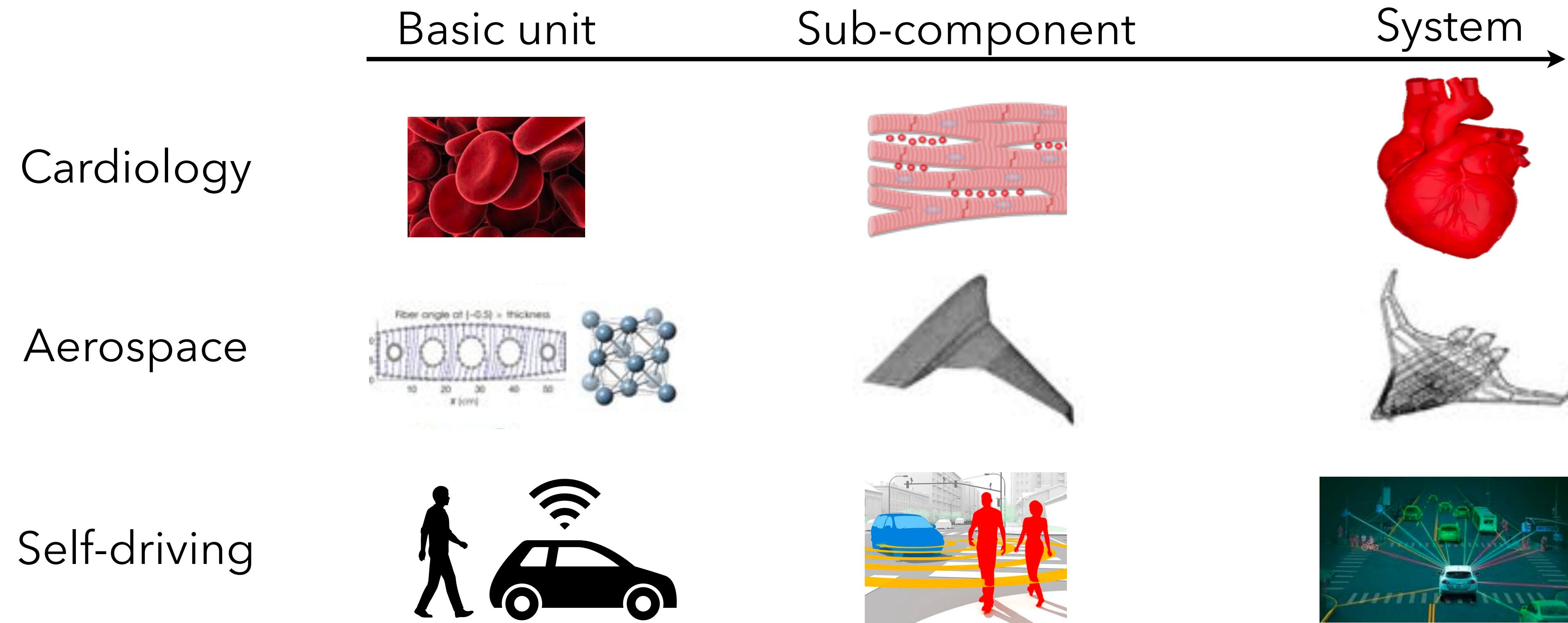
1. Use **real data** to infer decision's effect

Complex multi-scale simulation systems

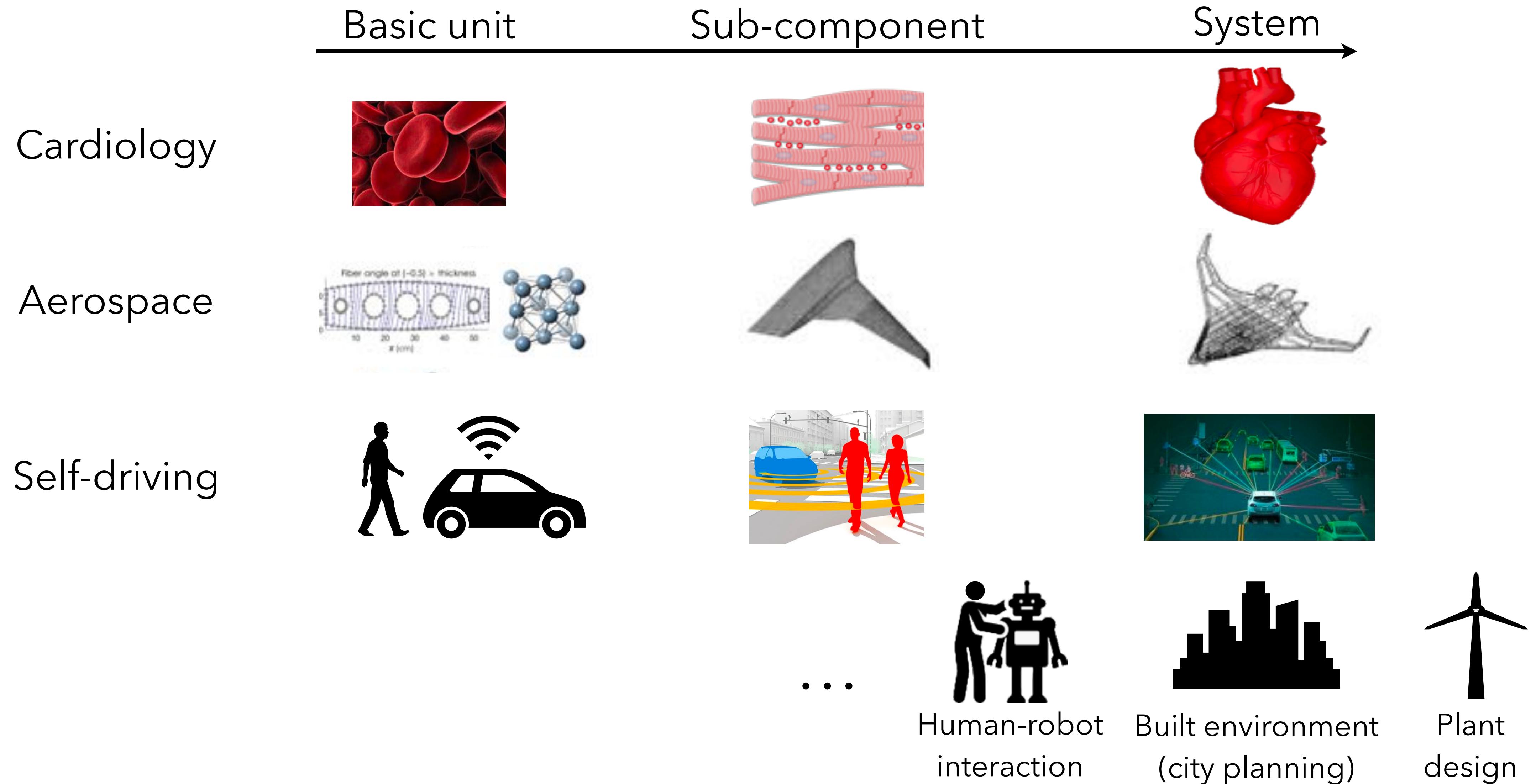
Complex multi-scale simulation systems



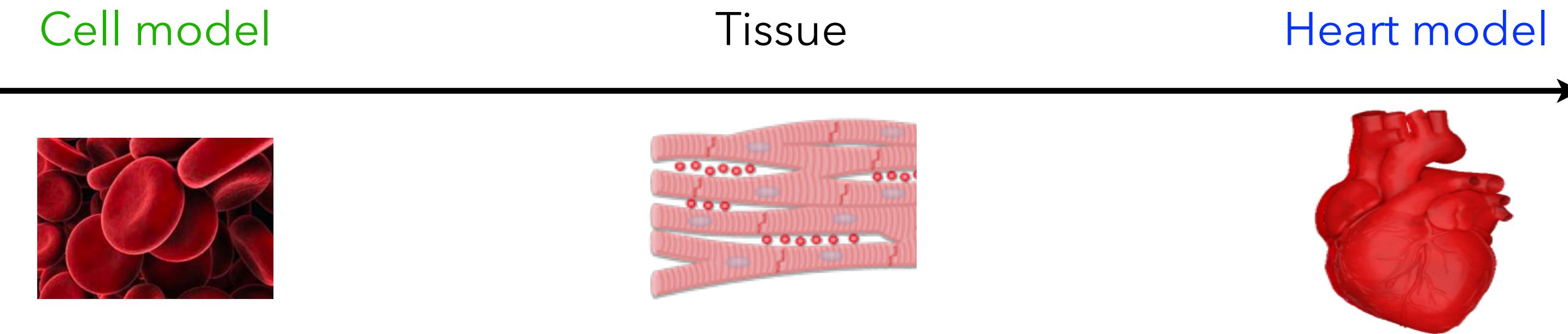
Complex multi-scale simulation systems



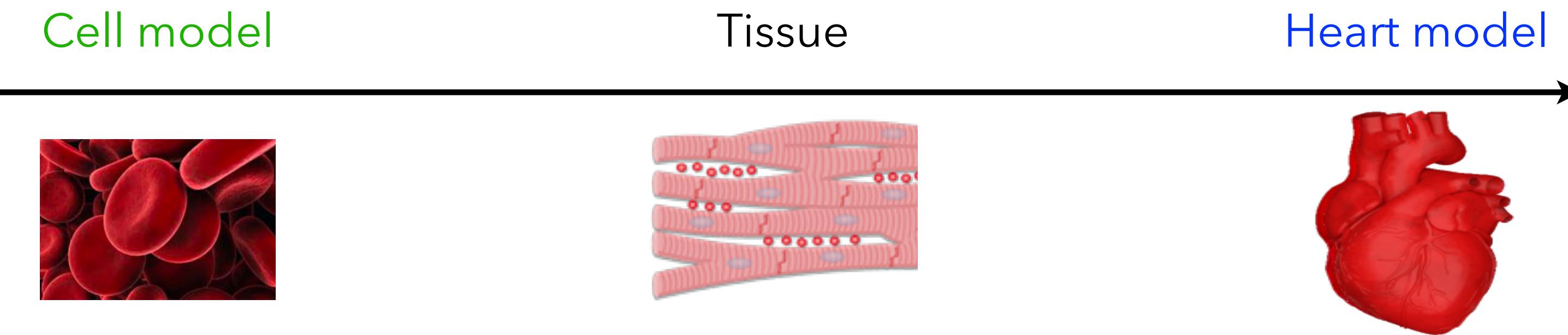
Complex multi-scale simulation systems



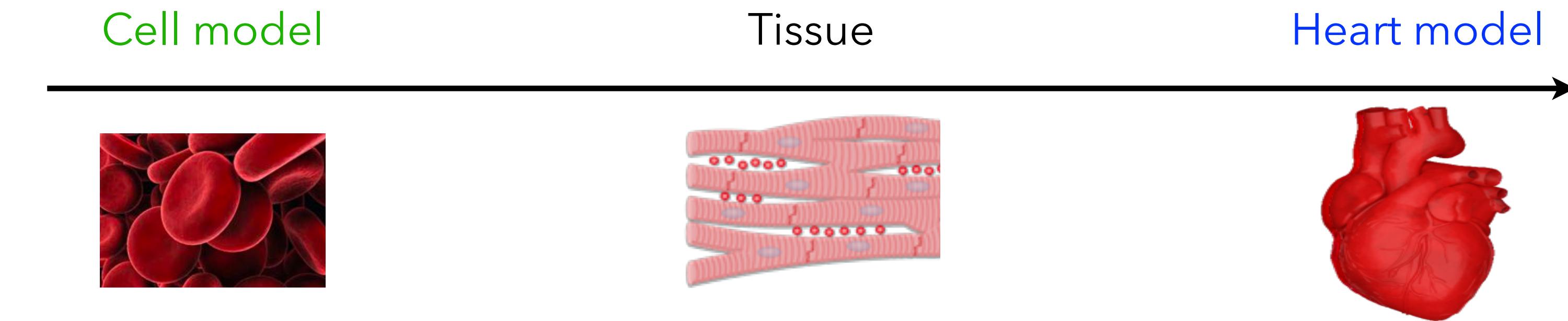
Computational cardiology: Personalized HeartBeats



Computational cardiology: Personalized HeartBeats



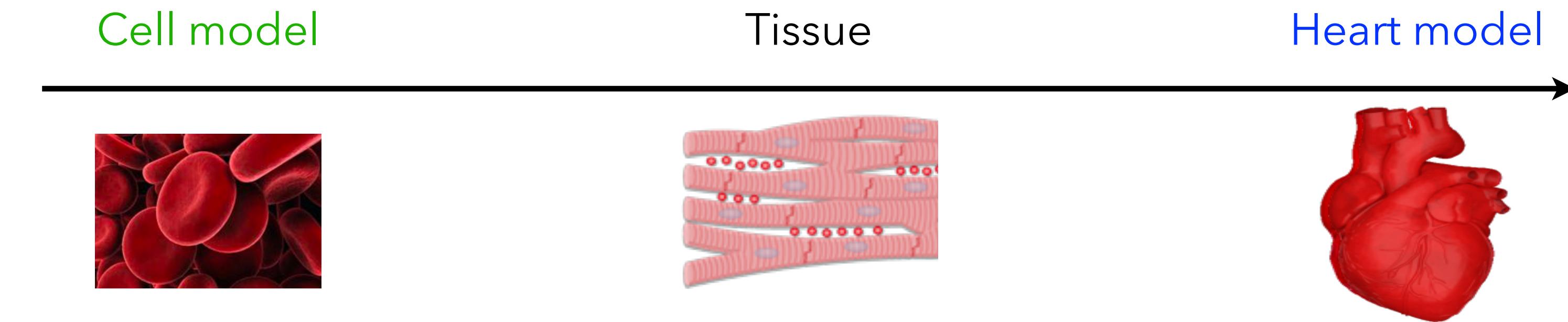
Computational cardiology: Personalized HeartBeats



gif credits
[alperdurmaz](#)

- Dysregulation of calcium signaling in heart cells can cause lethal arrhythmias

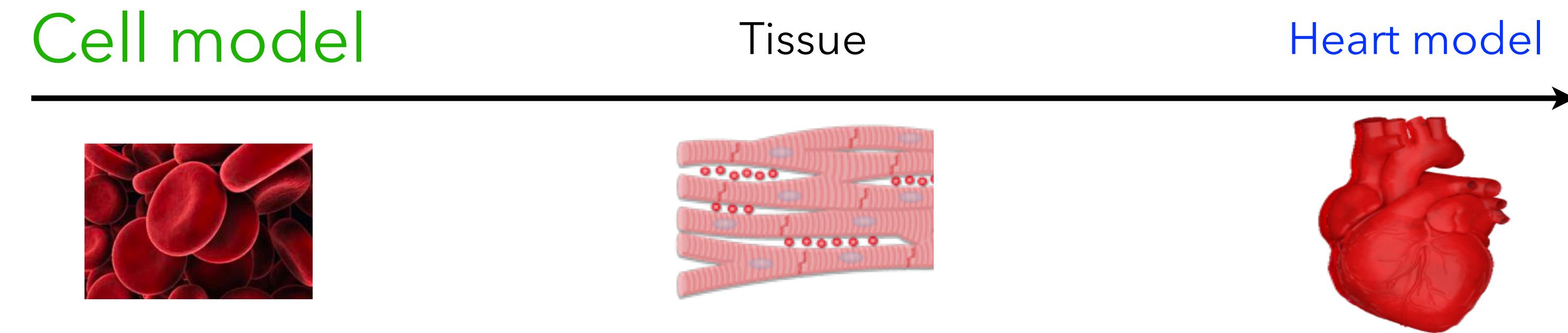
Computational cardiology: Personalized HeartBeats



gif credits
[alperdurmaz](#)

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- Task: **Simulate** multi-scale **digital twin** models of heart for **personalized predictions** of dysregulation's effect on a patient's heartbeat

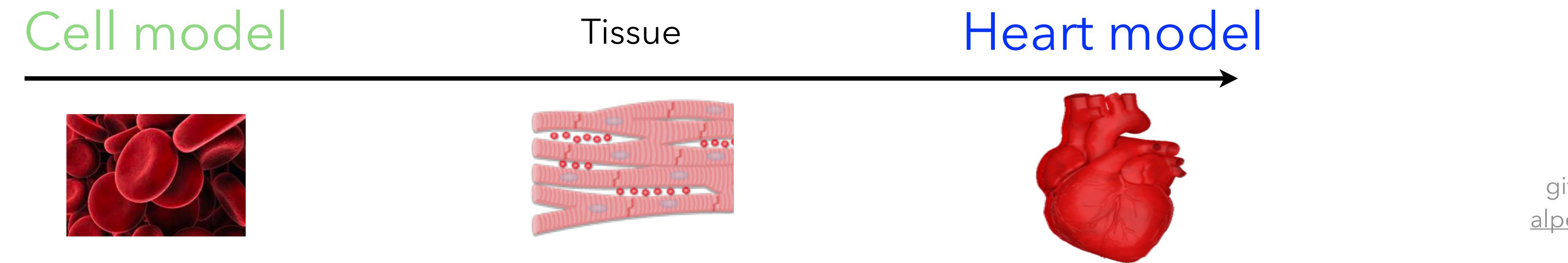
Computational cardiology: Personalized HeartBeats



gif credits
[alperdurmaz](#)

- Dysregulation of calcium signaling in heart cells can cause lethal arrhythmias
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Computational cardiology: Personalized HeartBeats



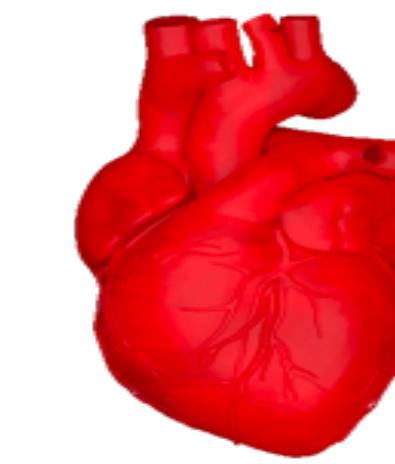
gif credits
[alperdurmaz](#)

- Dysregulation of calcium signaling in heart cells can cause lethal arrhythmias
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 1. **Estimate** cell-model parameters with uncertainty quantification with single cell measurements via Bayesian inference and posterior **sampling**
 2. **Propagate** cell-model **uncertainty** to whole-heart model via simulations and Monte Carlo **integration**

[Augustin+ '16, Colman '19, Riabiz+ '21, Niederer+ '21]

Impact of calcium signaling dysregulation on heartbeat— Two-stage inferential pipeline

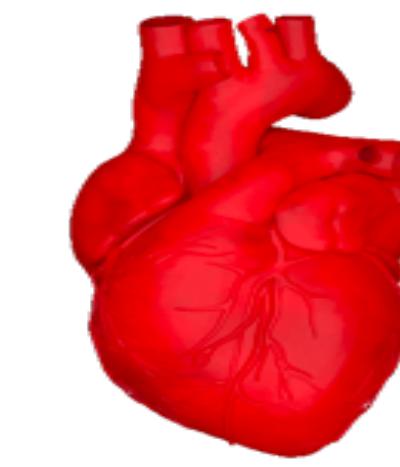
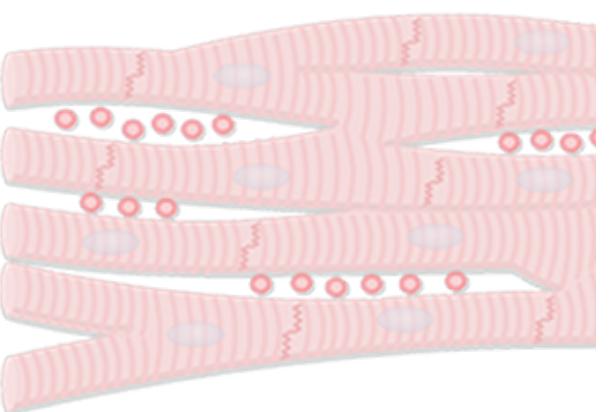
Cell
model X



Heart
model f

Impact of calcium signaling dysregulation on heartbeat— Two-stage inferential pipeline

Cell
model X



Heart
model f

1. Random sampling via MCMC

$$X_1, \dots, X_T \sim \mathbb{P}^*$$

(posterior in \mathbb{R}^{38})

Impact of calcium signaling dysregulation on heartbeat— Two-stage inferential pipeline

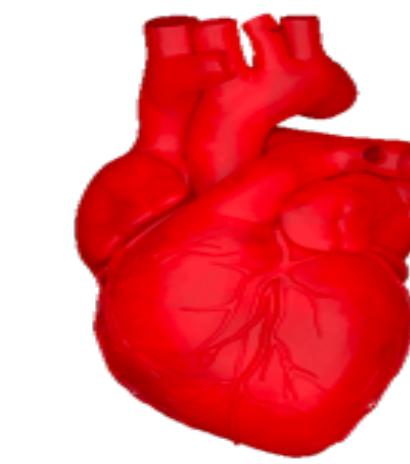
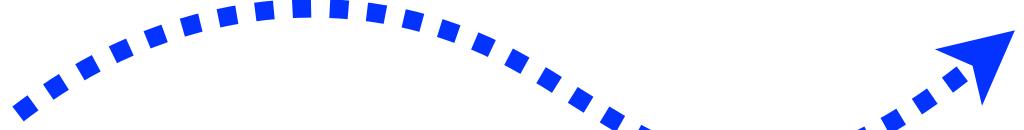
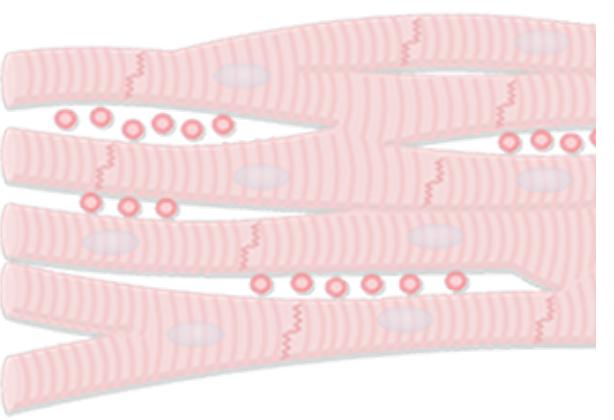
Cell
model X



1. Random sampling via MCMC

$$X_1, \dots, X_T \sim \mathbb{P}^{\star}$$

(posterior in \mathbb{R}^{38})



Heart
model f

2. Uncertainty propagation via Monte Carlo integration (mean, variance,...)

$$\mathbb{P}^{\star}f \triangleq \int f(X) d\mathbb{P}^{\star}(X) \approx \frac{1}{T} \sum_{i=1}^T f(X_i)$$

Standard tasks but computationally challenging...

Cell
model X

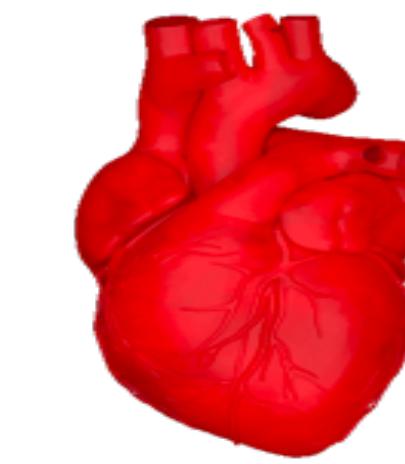


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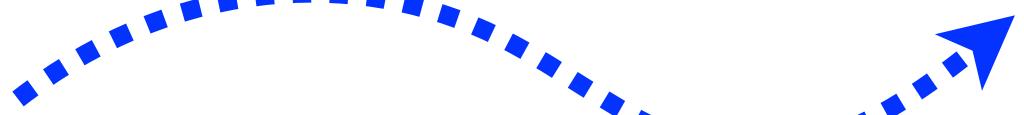
- $T = 10^6$ to explore \mathbb{P}^* well



Heart
model f

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$$\mathbb{P}^* f \triangleq \int f(X) d\mathbb{P}^*(X) \approx \frac{1}{T} \sum_{i=1}^T f(X_i)$$



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Cell
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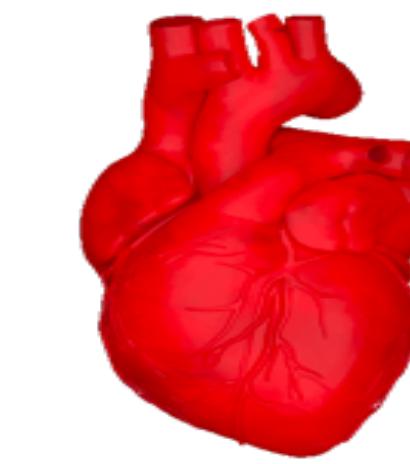


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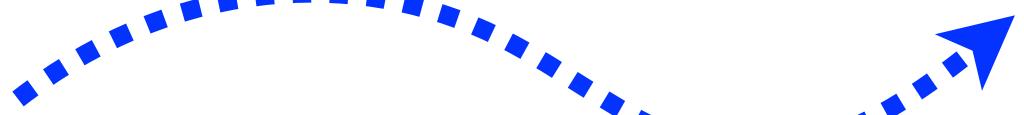
- $T = 10^6$ to explore \mathbb{P}^* well
- Time to run **MCMC**
~ 2 CPU weeks



Heart
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Cell
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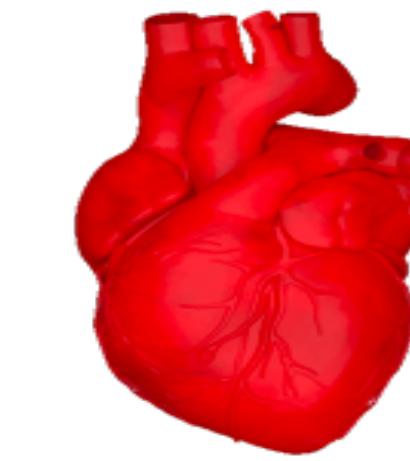
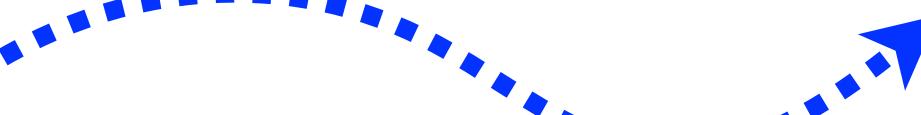
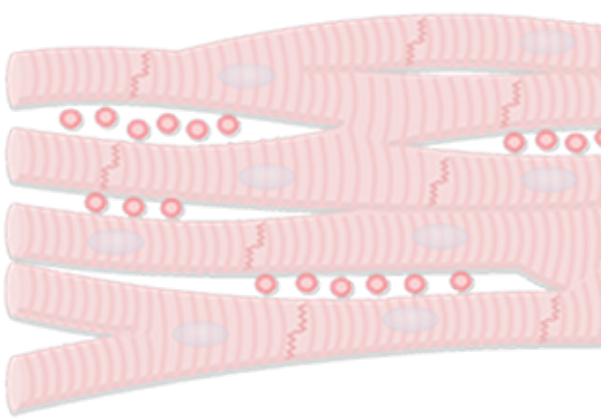


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Heart
model f

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- Single f simulation ~ 4 CPU weeks

Standard tasks but computationally challenging...

Cell
model X

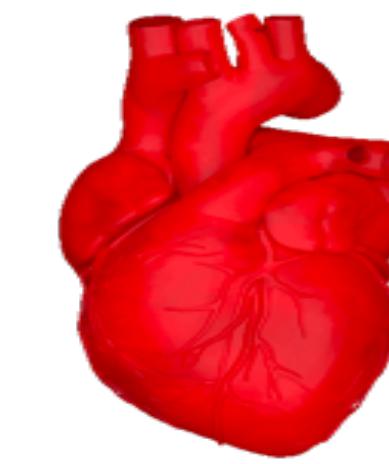
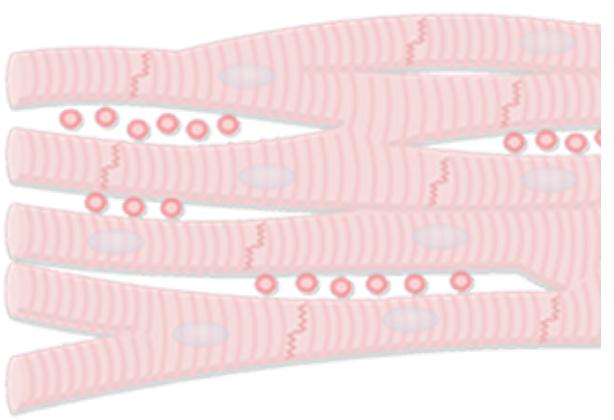


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Heart
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- Time to compute **sample mean**
~ 4 Million CPU weeks

Standard tasks but computationally challenging...

Cell
model X

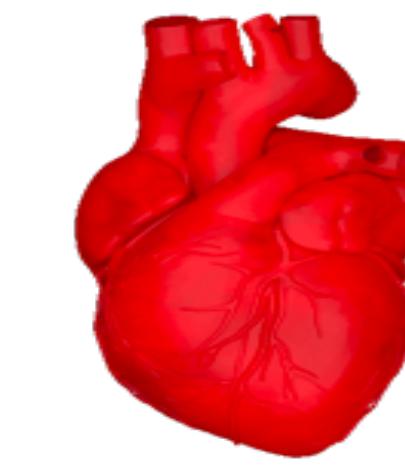


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(posterior in \mathbb{R}^{38})

- $T = 10^6$ to explore \mathbb{P}^* well
- Time to run **MCMC**
~ 2 CPU weeks
- **How to make MCMC computationally faster?**



Heart
model f

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$$\mathbb{P}^* f \triangleq \int f(X) d\mathbb{P}^*(X) \approx \frac{1}{T} \sum_{i=1}^T f(X_i)$$

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~ 4 Million CPU weeks
- **How to make integration computationally feasible?**

Part 2 overview: Computationally-efficient integration for high-dimensional models

Cell
model X

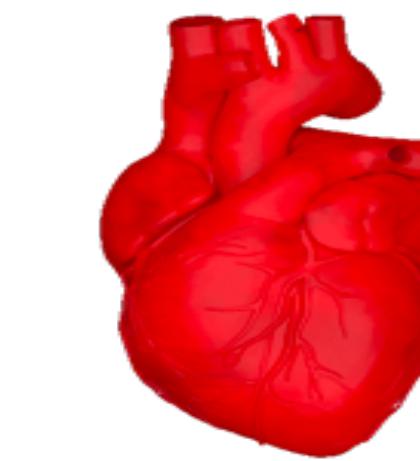


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Heart
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 ~ 4 Million CPU weeks
- **How to make integration computationally feasible?**

??

This talk

Efficient integration via distribution compression

Efficient integration via distribution compression

$\textcolor{blue}{T}$ IID or MCMC points

$$X_1, \dots, X_T$$

$$\mathbb{P}_T f \triangleq \frac{\sum_{i=1}^T f(X_i)}{T}$$

Efficient integration via distribution compression

T IID or MCMC points

s output points (coreset)

$$X_1, \dots, X_T$$

Compress

$$X'_1, \dots, X'_s$$

$$\mathbb{P}_T f \triangleq \frac{\sum_{i=1}^T f(X_i)}{T}$$

$$\mathbb{P}_{out} f \triangleq \frac{\sum_{i=1}^s f(X'_i)}{s}$$

s (fewer) function evaluations

Efficient integration via distribution compression

$\textcolor{blue}{T}$ IID or MCMC points

$\textcolor{violet}{s}$ output points (coreset)

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Compress

$$X'_1, \dots, X'_s$$

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$$\mathbb{P}_{out} f \triangleq \frac{\sum_{i=1}^s f(X'_i)}{s}$$

s (fewer) function evaluations

$$|\mathbb{P}^\star f - \mathbb{P}_T f| = \Theta(\textcolor{blue}{T}^{-1/2})$$

Efficient integration via distribution compression

T IID or MCMC points

s output points (coreset)

$$X_1, \dots, X_T$$

Compress

$$X'_1, \dots, X'_s$$

$$\mathbb{P}_T f \triangleq \frac{\sum_{i=1}^T f(X_i)}{T}$$

$$\mathbb{P}_{out} f \triangleq \frac{\sum_{i=1}^s f(X'_i)}{s}$$

s (fewer) function evaluations

Standard thinning

(take every T/s -th point)

or iid thinning/

uniform **sub-sampling**

$$|\mathbb{P}^\star f - \mathbb{P}_T f| = \Theta(T^{-1/2})$$

$$|\mathbb{P}^\star f - \mathbb{P}_{out} f| = \Theta(s^{-1/2})$$

$$|\mathbb{P}^\star f - \mathbb{P}_{out} f| = \Theta(T^{-1/4})$$

when $s = T^{1/2}$

a million \rightarrow a thousand

T IID or MCMC points

a million → a thousand

$T^{1/2}$ output points

$$|\mathbb{P}^{\star}f - \mathbb{P}_T f| = \Theta(T^{-1/2})$$

Standard thinning
→

$$|\mathbb{P}^{\star}f - \mathbb{P}_{out} f| = \Theta(T^{-1/4})$$

What is the best error we can hope for?

T IID or MCMC points

a million → a thousand

$T^{1/2}$ output points

$$|\mathbb{P}^{\star}f - \mathbb{P}_T f| = \Theta(T^{-1/2}) \xrightarrow{\text{Standard thinning}} |\mathbb{P}^{\star}f - \mathbb{P}_{out} f| = \Theta(T^{-1/4})$$

What is the best error we can hope for?

T IID or MCMC points

a million → a thousand

$T^{1/2}$ output points

$$|\mathbb{P}^{\star}f - \mathbb{P}_T f| = \Theta(T^{-1/2}) \xrightarrow{\text{Standard thinning}} |\mathbb{P}^{\star}f - \mathbb{P}_{out} f| = \Theta(T^{-1/4})$$

$\Omega(T^{-1/2})$ minimax **lower bound**

- If output = $T^{1/2}$ points
- If input = T IID points (any estimator)

[Tolstikhin+ '17, Philips+ '20]

Prior strategies for efficient integration

T IID or MCMC points

a million → a thousand

$T^{1/2}$ output points

$$|\mathbb{P}^{\star}f - \mathbb{P}_T f| = \Theta(T^{-1/2}) \xrightarrow{\text{Standard thinning}} |\mathbb{P}^{\star}f - \mathbb{P}_{out} f| = \Theta(\textcolor{red}{T^{-1/4}})$$

$\Omega(\textcolor{blue}{T^{-1/2}})$ minimax lower bound

Prior strategies for efficient integration

T IID or MCMC points

a million → a thousand

$T^{1/2}$ output points

$$|\mathbb{P}^{\star}f - \mathbb{P}_T f| = \Theta(T^{-1/2}) \xrightarrow{\text{Standard thinning}} |\mathbb{P}^{\star}f - \mathbb{P}_{out} f| = \Theta(T^{-1/4})$$

Special \mathbb{P}^{\star}
-Uniform on $[0,1]^d$
-Bounded support &
special function class

- $o(T^{-1/4})$ error guarantee:
Quasi Monte Carlo, Bayesian quadrature,
determinantal point processes, Haar thinning
[O'Hagan '91, Hickernell '98, Novak+'10, Liu+'18,
Karvonen+'18, Dwivedi+'19, Belhadji+'20]

$\Omega(T^{-1/2})$ minimax lower bound

Prior strategies for efficient integration

T IID or MCMC points

a million → a thousand

$T^{1/2}$ output points

$$|\mathbb{P}^{\star}f - \mathbb{P}_T f| = \Theta(T^{-1/2})$$

Standard thinning

$$|\mathbb{P}^{\star}f - \mathbb{P}_{out} f| = \Theta(T^{-1/4})$$

Special \mathbb{P}^{\star}

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[O'Hagan '91, Hickernell '98, Novak+'10, Liu+'18,
Karvonen+'18, Dwivedi+'19, Belhadji+'20]

Generic \mathbb{P}^{\star} & rich function class

$\tilde{O}(T^{-1/4})$ error guarantee:
Kernel herding, greedy sign selection, Stein
points MCMC, support points, supersampling
[Chen+'10, Lacoste+'15, Paige+'16, Tolstikhin+'17,
Mak+'18, Chen '19, Karnin '19]

$\Omega(T^{-1/2})$ minimax lower bound

T IID or MCMC points

a million \rightarrow a thousand

$T^{1/2}$ output points

$$|\mathbb{P}^{\star}f - \mathbb{P}_T f| = \Theta(T^{-1/2})$$

Standard thinning
→

$$|\mathbb{P}^{\star}f - \mathbb{P}_{out} f| = \Theta(\textcolor{red}{T}^{-1/4})$$

$\Omega(\textcolor{blue}{T}^{-1/2})$ minimax lower bound

A new practical & provably near-optimal procedure

T IID or MCMC points

a million → a thousand

$T^{1/2}$ output points

$$|\mathbb{P}^{\star}f - \mathbb{P}_T f| = \Theta(T^{-1/2})$$



$$|\mathbb{P}^{\star}f - \mathbb{P}_{out} f| = \Theta(T^{-1/4})$$



Kernel thinning

Dwivedi and Mackey '21, '22

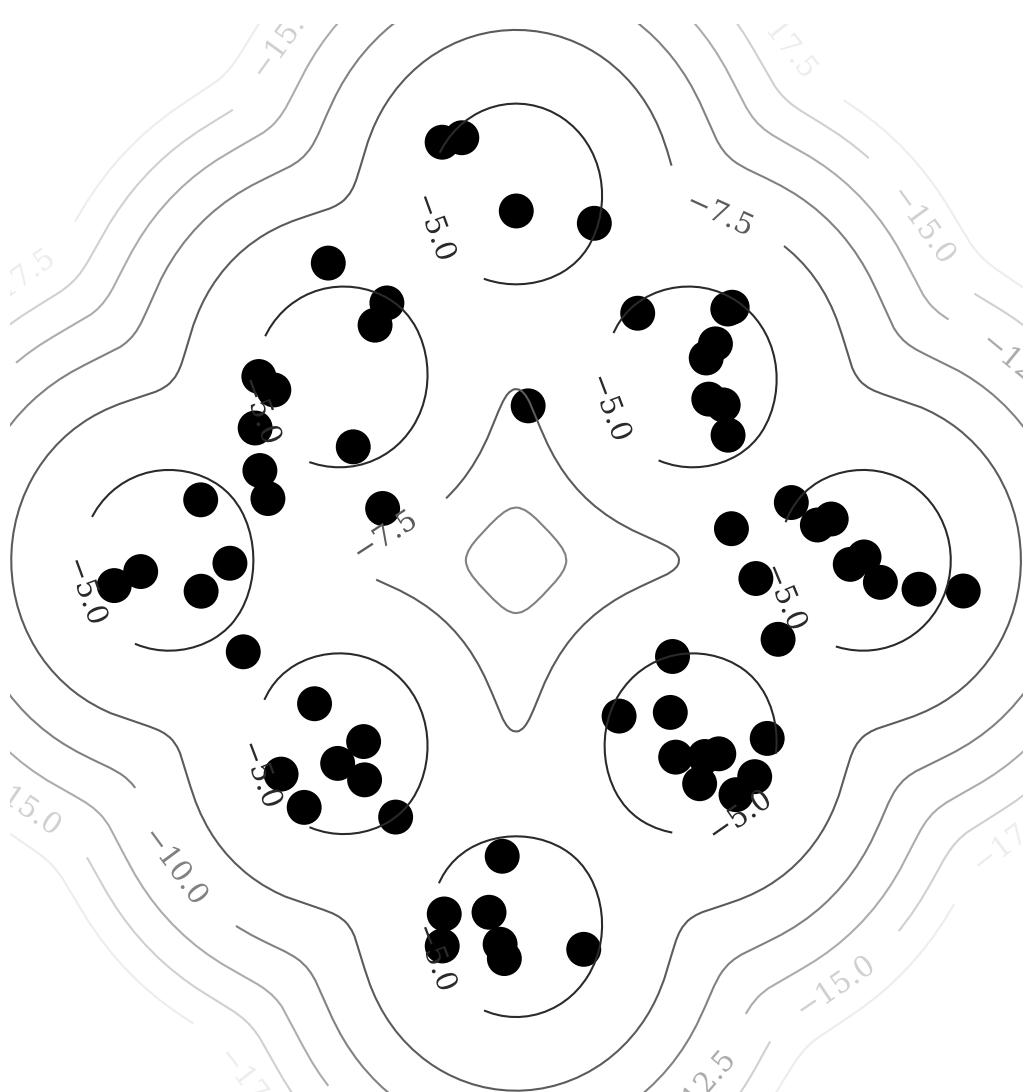
$$|\mathbb{P}^{\star}f - \mathbb{P}_{out} f| = \tilde{O}(T^{-1/2})$$

- ✓ for generic \mathbb{P}^{\star} on generic domains
- ✓ for rich function classes

$\Omega(T^{-1/2})$ minimax lower bound

Visual comparison on $P^* = 8$ mixture of Gaussian

64 iid input points



Standard thinning



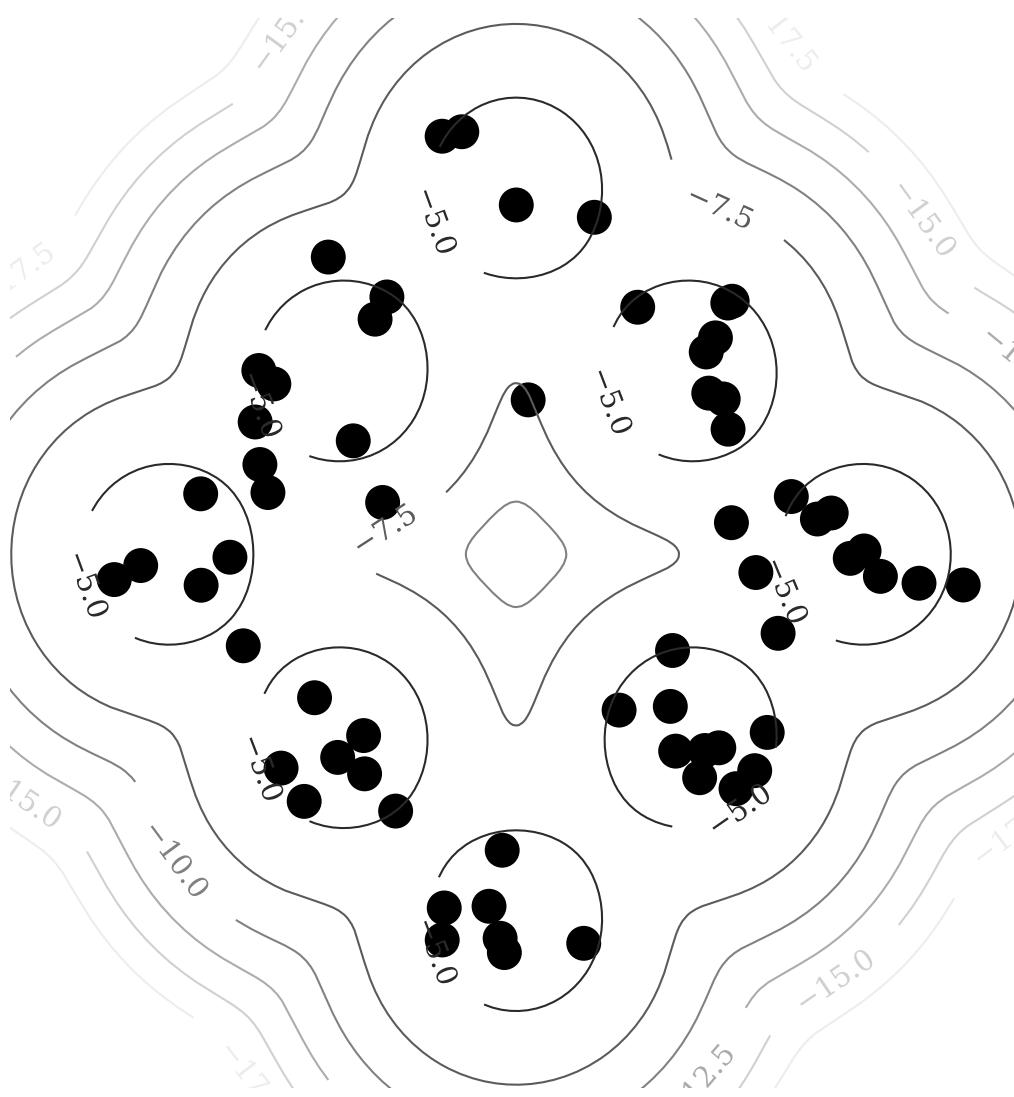
8 output points

Kernel thinning



Visual comparison on $P^* = 8$ mixture of Gaussian

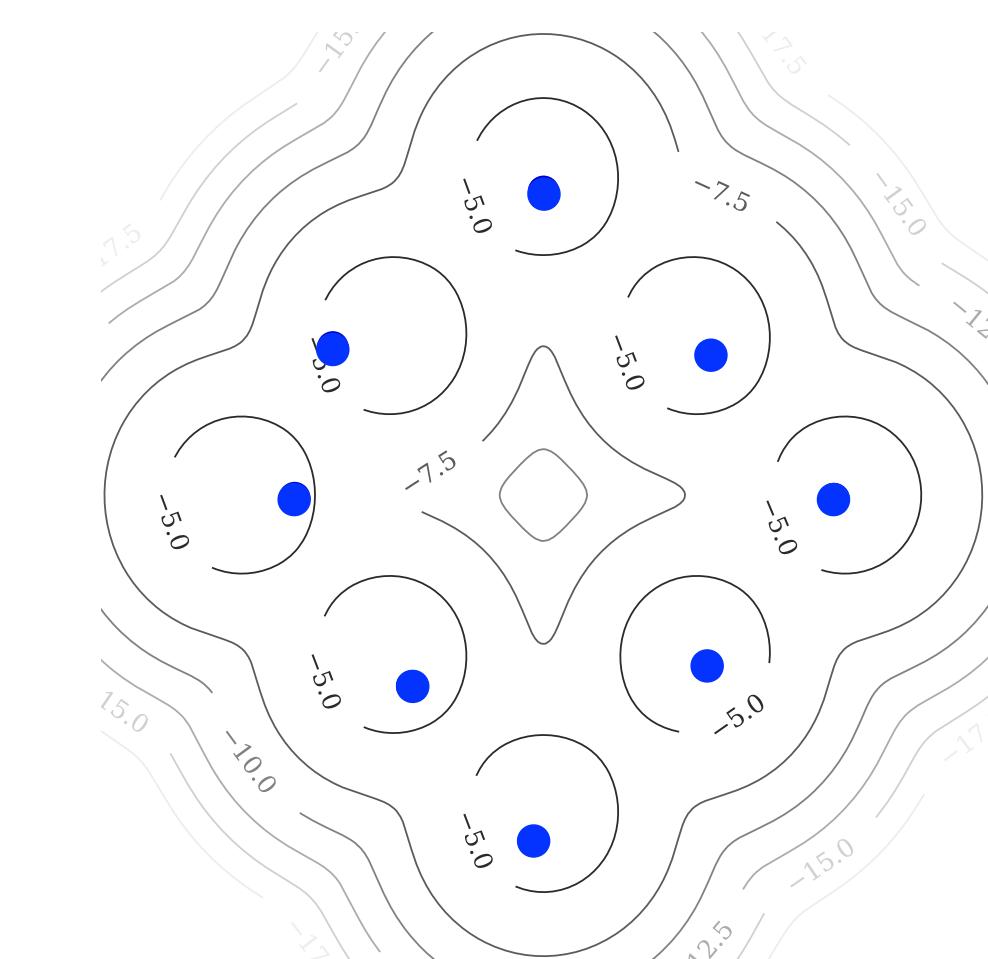
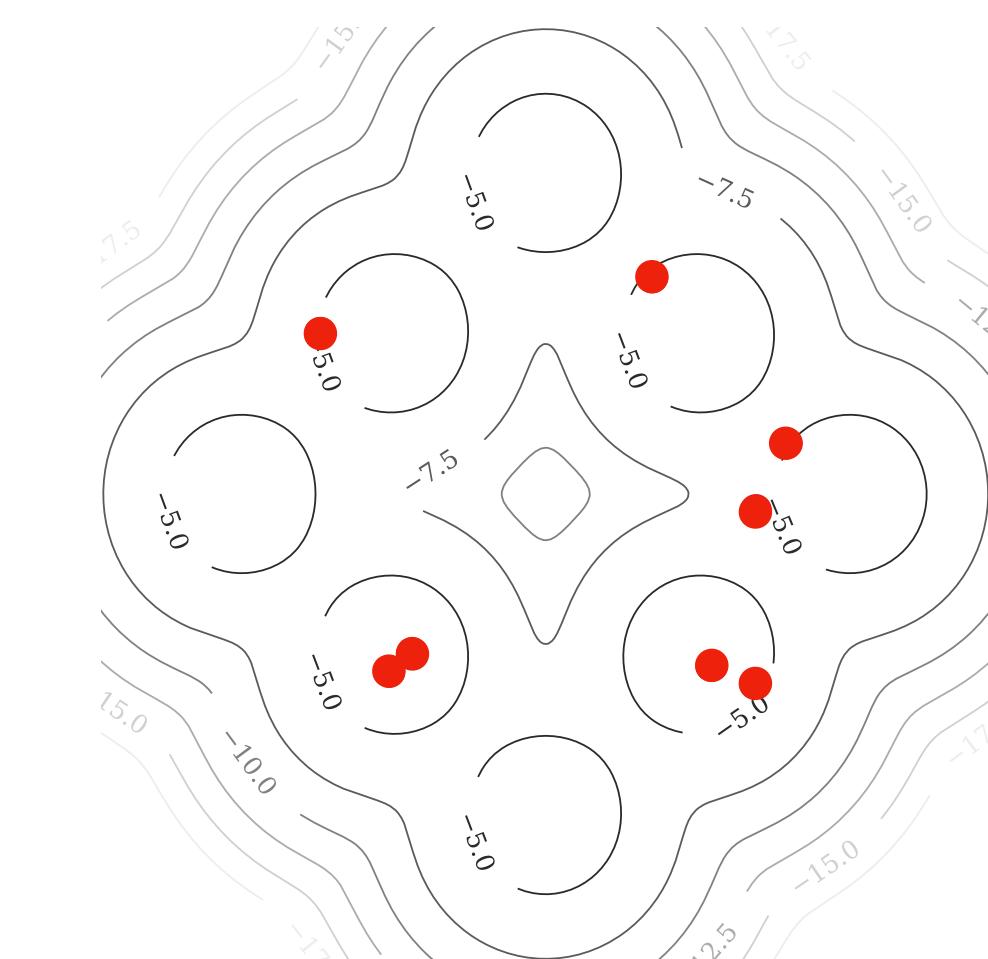
64 iid input points



Standard thinning

Kernel thinning

8 output points



Quantitative measure: **Worst-case error** over a rich class

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Namely, over the unit ball of a reproducing kernel Hilbert space (RKHS)

$$\sup_{\|f\|_k \leq 1} |\mathbb{P}^\star f - \mathbb{P}_{out} f|$$

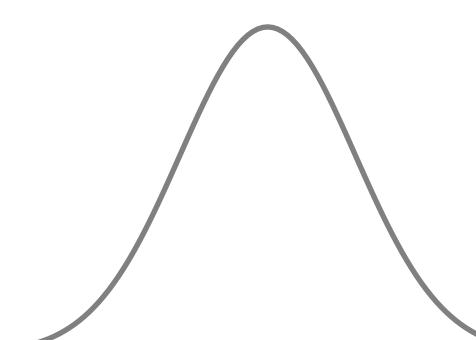
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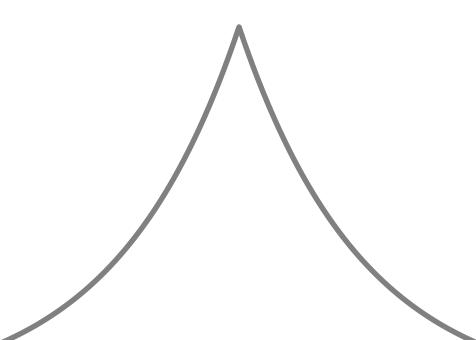
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- Parameterized by a reproducing kernel \mathbf{k}
any symmetric ($\mathbf{k}(x, y) = \mathbf{k}(y, x)$) and positive semidefinite function

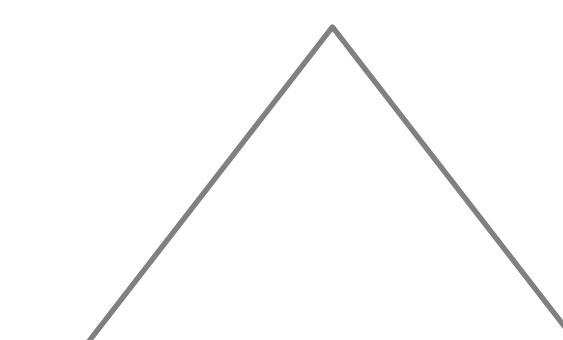
Gaussian



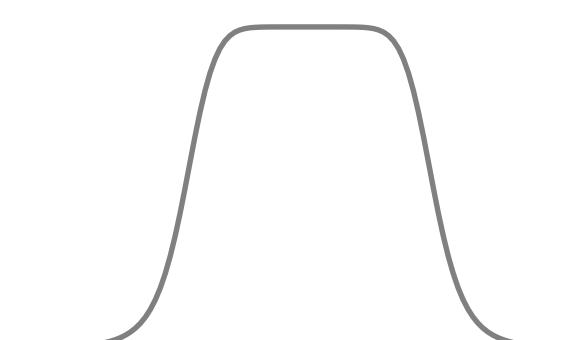
Matérn



Bspline



Inverse multiquadric



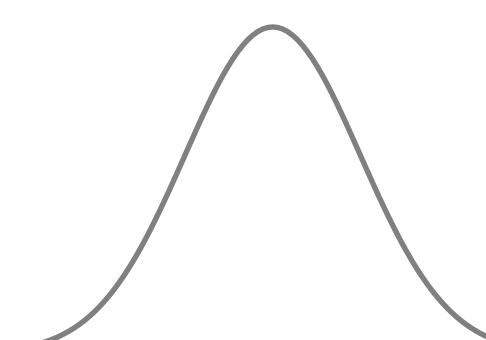
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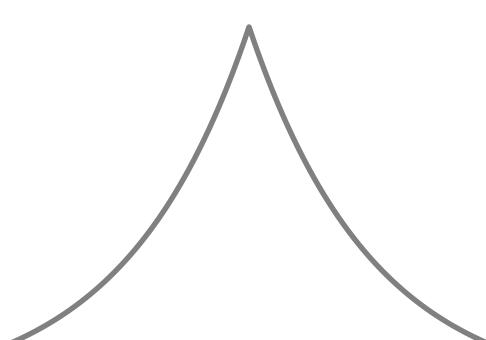
$$\sup_{\|f\|_k \leq 1} |\mathbb{P}^{\star} f - \mathbb{P}_{out} f|$$

- Parameterized by a reproducing kernel k
any symmetric ($k(x, y) = k(y, x)$) and positive semidefinite function
- **Metrizes convergence in distribution** for popular infinite-dimensional k

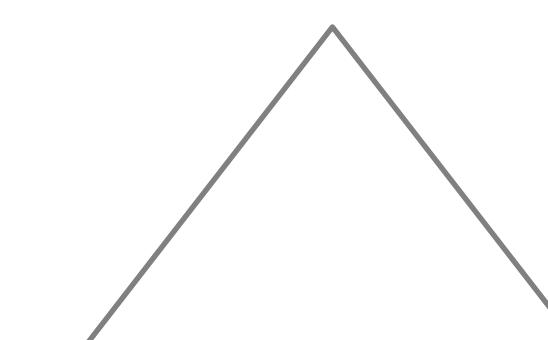
Gaussian



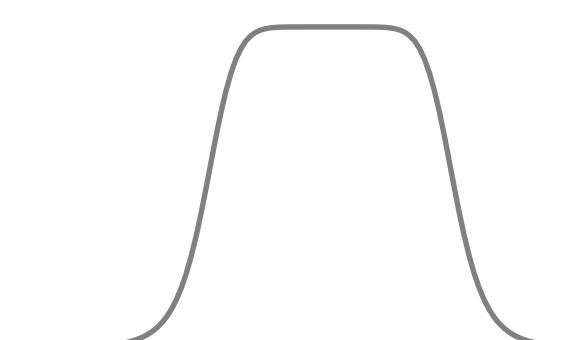
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Bspline



Inverse multiquadric



Main result: A high probability bound for generic \mathbb{P}^* and k

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Informal theorem: [Dwivedi and Mackey'21, '22 and Dwivedi-Shetty-Mackey '22]

Kernel thinning uses $O(T \log^3 T)$ **kernel evaluations** to output $T^{1/2}$ points, that with high probability satisfy

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- $|\mathbb{P}^*f - \mathbb{P}_{out}f| \lesssim \sqrt{\frac{\log T}{T}} \cdot \|f\|_{\mathbf{k}} \sqrt{\|\mathbf{k}\|_{\infty}}$ for a fixed f in the RKHS of \mathbf{k} (any kernel)
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- A near-quadratic gain over $T^{-1/4}$ standard thinning error

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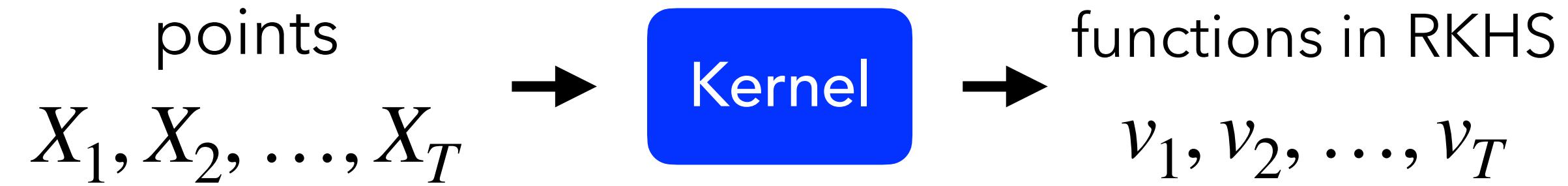
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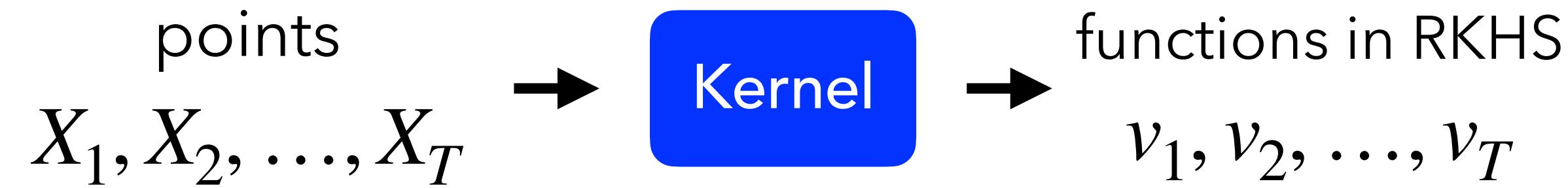
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- $\sup_{\|f\|_{\mathbf{k}} \leq 1} |\mathbb{P}^*f - \mathbb{P}_{out}f| \lesssim \sqrt{\frac{\log^{d/2+1} T}{T}}$ Sub-gaussian \mathbb{P}^* and \mathbf{k} on \mathbb{R}^d (Gaussian)
 $\lesssim \sqrt{\frac{\log^{d+1} T}{T}}$ Sub-exponential \mathbb{P}^* and \mathbf{k} on \mathbb{R}^d (Matérn)

- A near-quadratic gain over $T^{-1/4}$ standard thinning error
- Matches minimax lower bounds $T^{-1/2}$ up to log factors

Kernel thinning



Kernel thinning \equiv Recursive halving via kernel evaluations



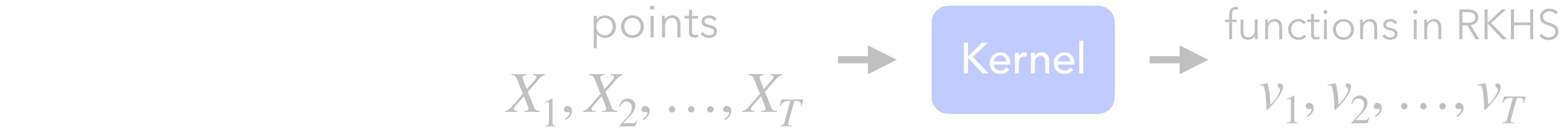
Kernel halving



$v_1, v_2, \dots, v_T \xrightarrow{\text{Kernel halving}} v'_1, v'_2, \dots, v'_{T/2}$

$$\left| \frac{\sum_{i=1}^T v_i}{T} - \frac{\sum_{i=1}^{T/2} v'_i}{T/2} \right| = \text{small}$$

Kernel halving \equiv Discrepancy minimization problem



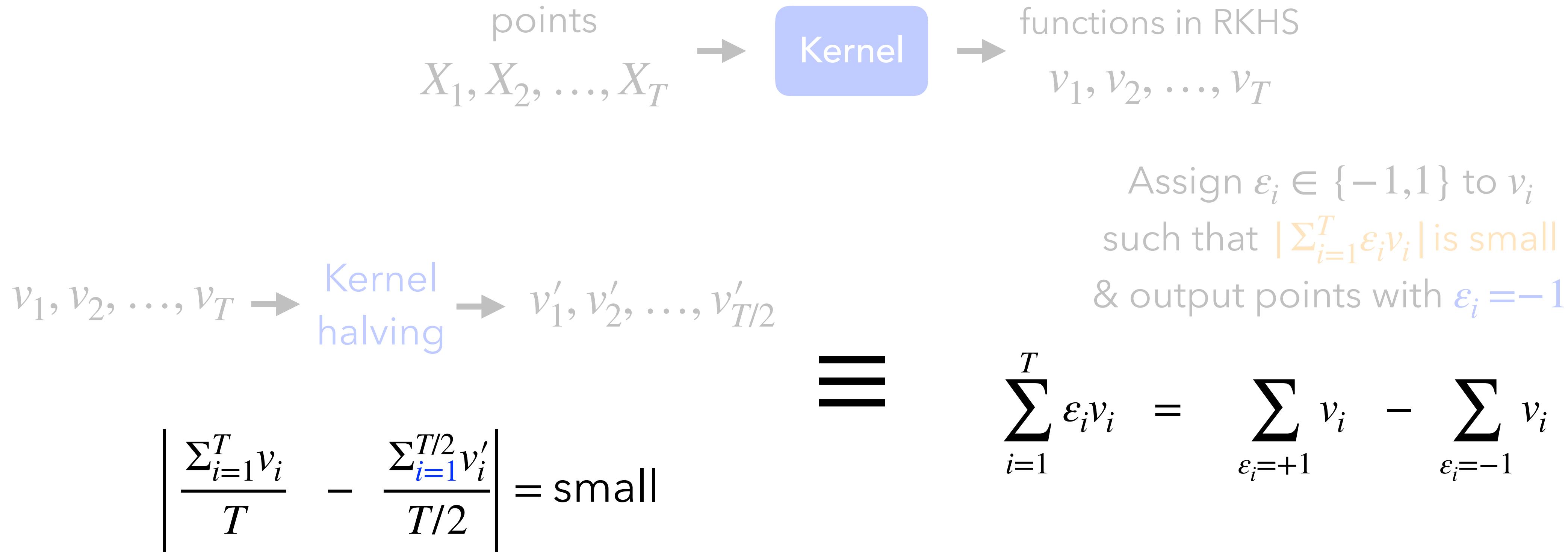
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\equiv

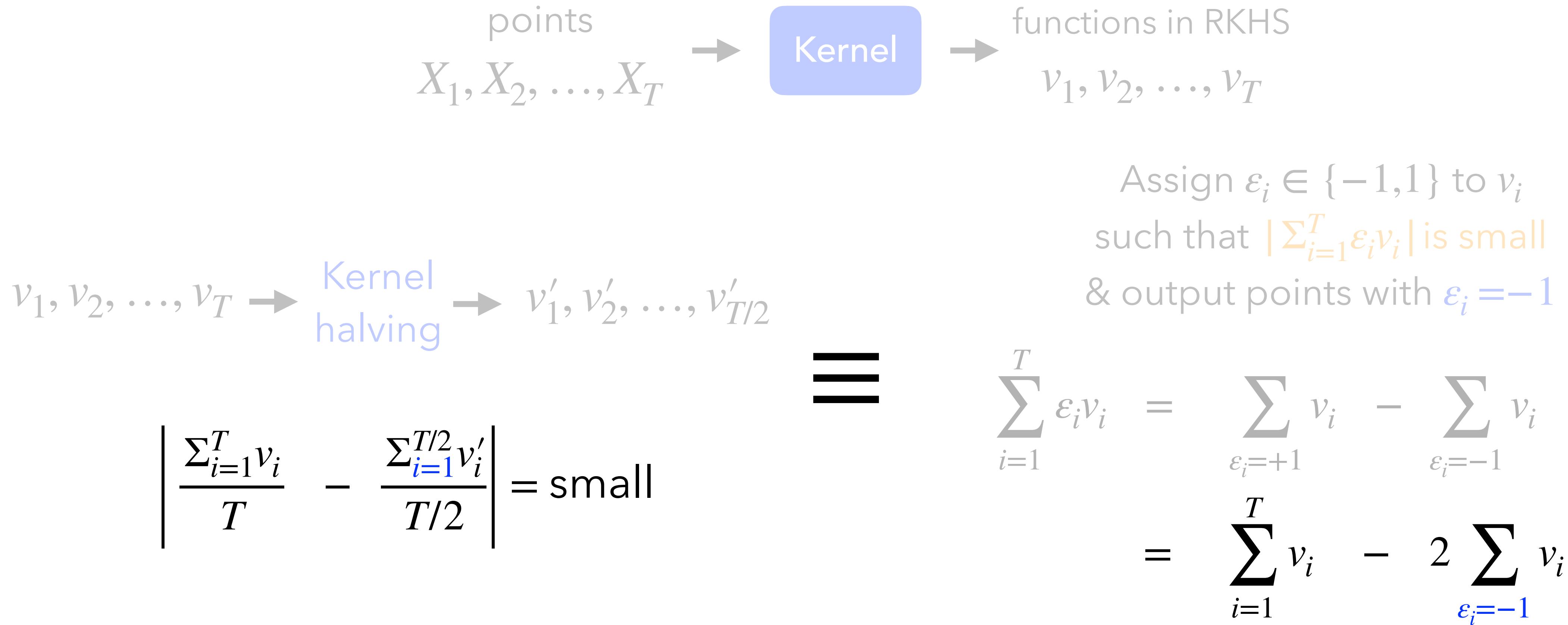
$$\left| \frac{\sum_{i=1}^T v_i}{T} - \frac{\sum_{i=1}^{T/2} v'_i}{T/2} \right| = \text{small}$$

Assign $\varepsilon_i \in \{-1, 1\}$ to v_i
such that $|\sum_{i=1}^T \varepsilon_i v_i|$ is small
& output points with $\varepsilon_i = -1$

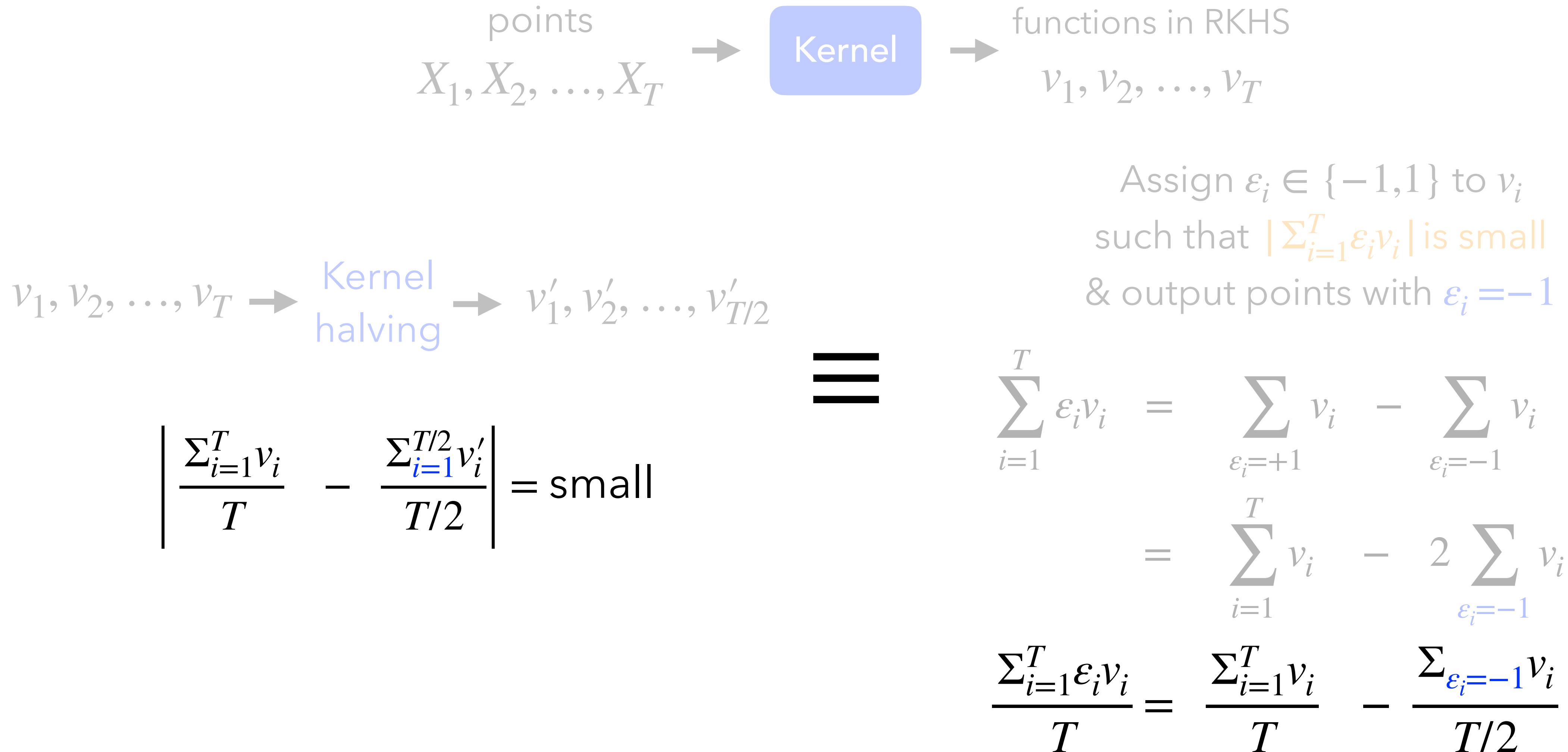
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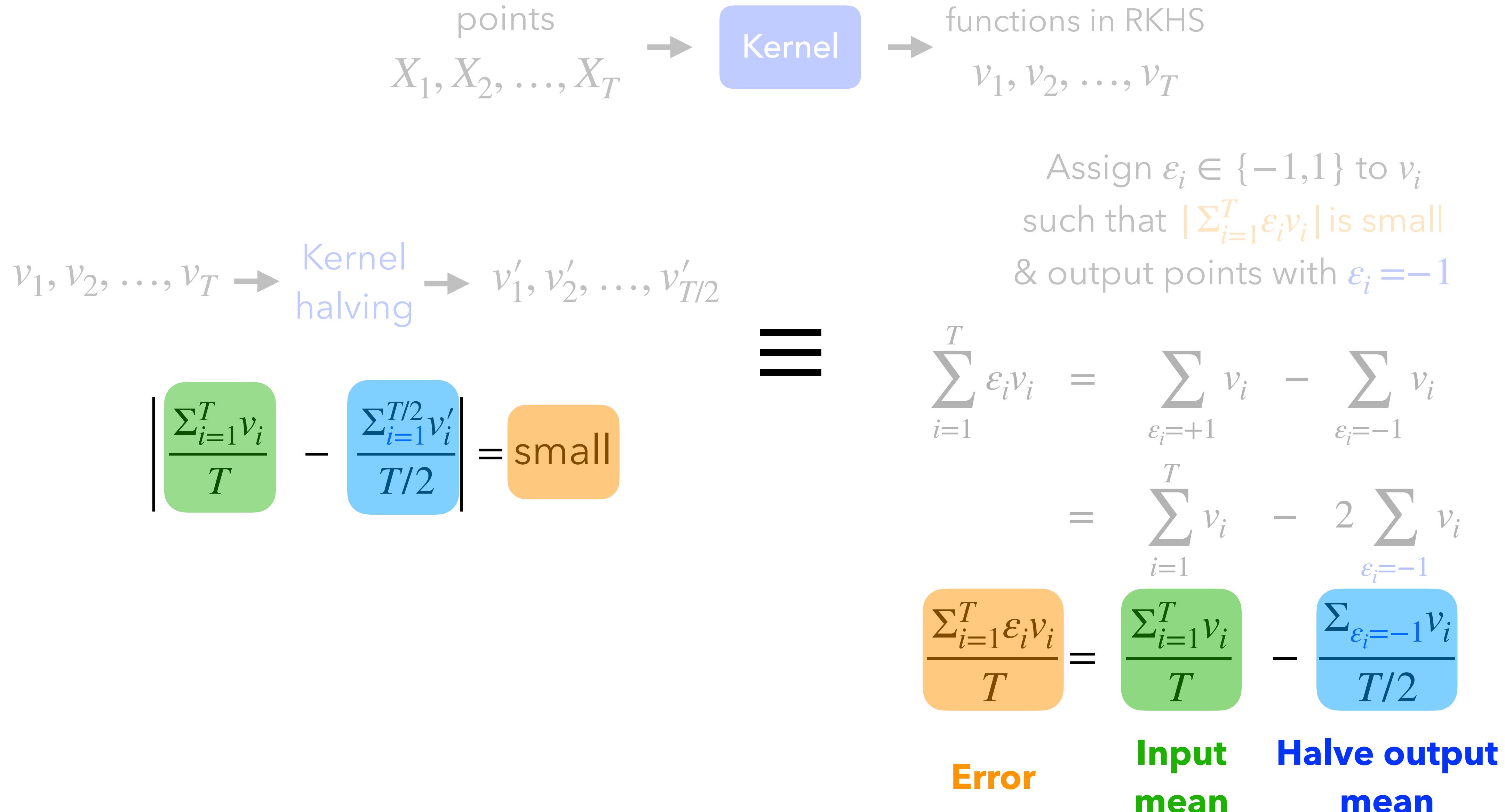
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Kernel thinning



Discrepancy minimization

[... Spencer '77, Banaszczyk '98, '12, Eldan+ '18, ...
Bansal+ '16, '18, '19, '20, Dwivedi+ '19, Alweiss+ '21, ...]

Is KT better practically? Gaussian P^* in \mathbb{R}^d

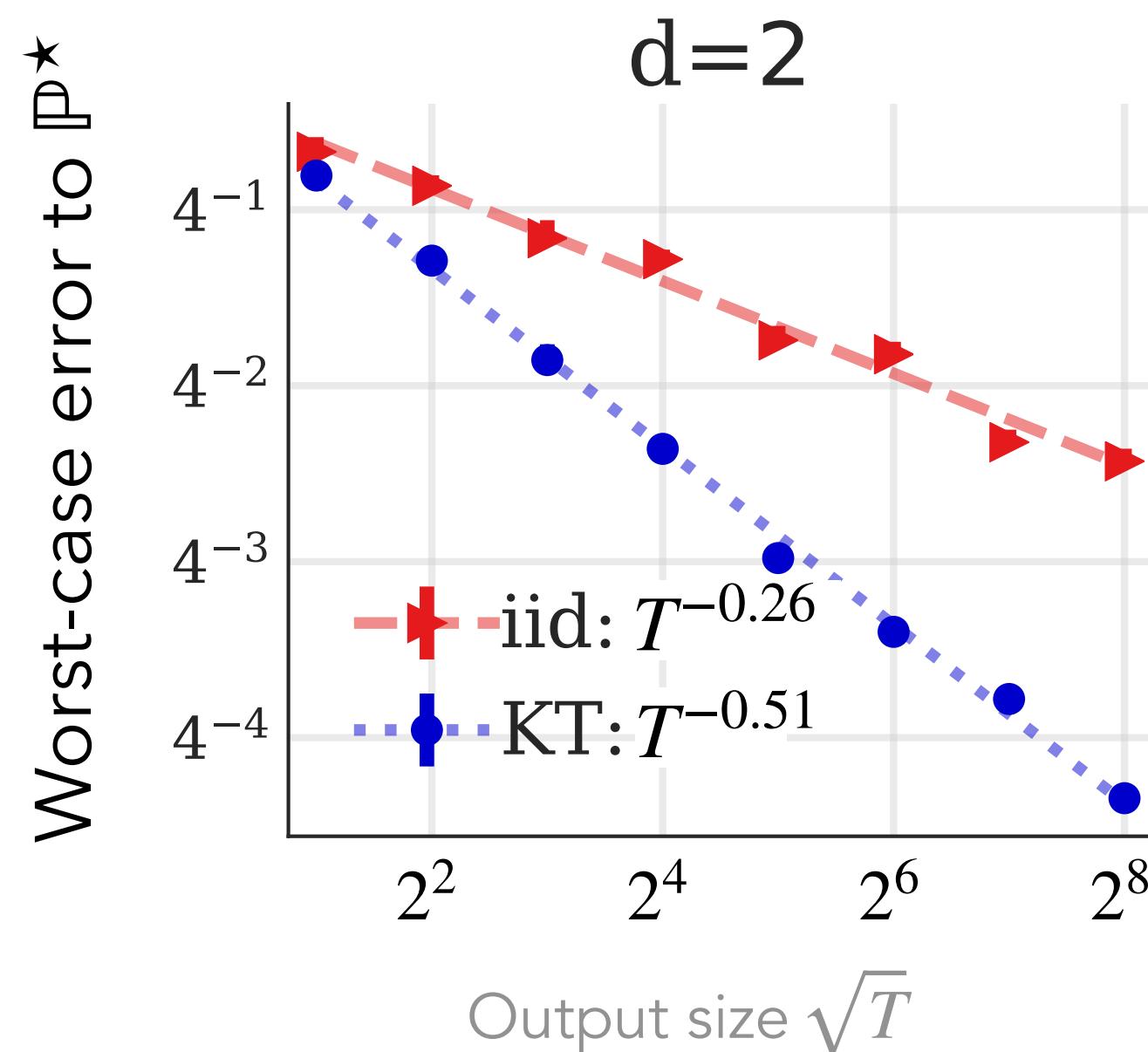
iid input, Gaussian kernel

Worst-case error to P^*

Output size \sqrt{T}

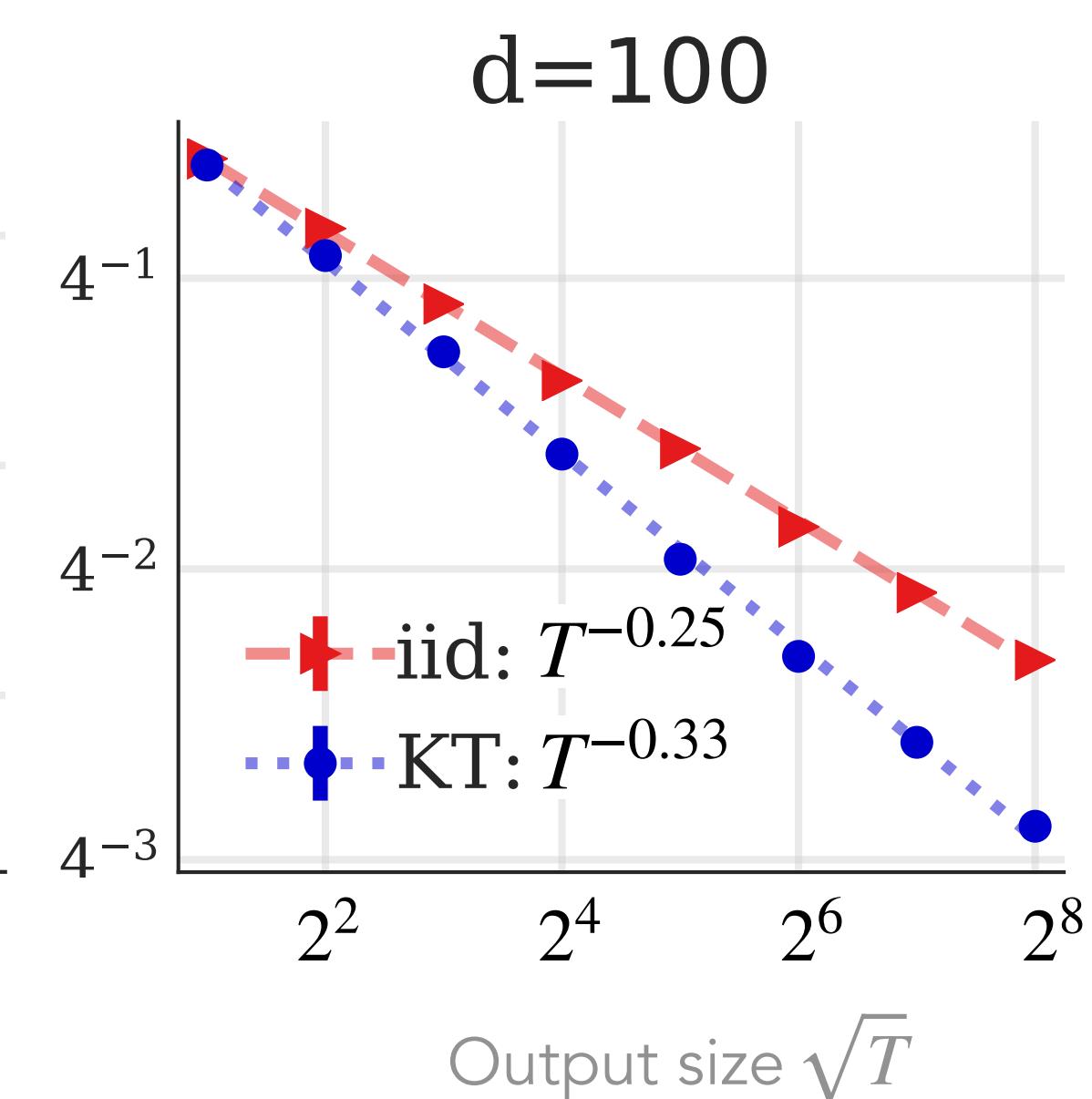
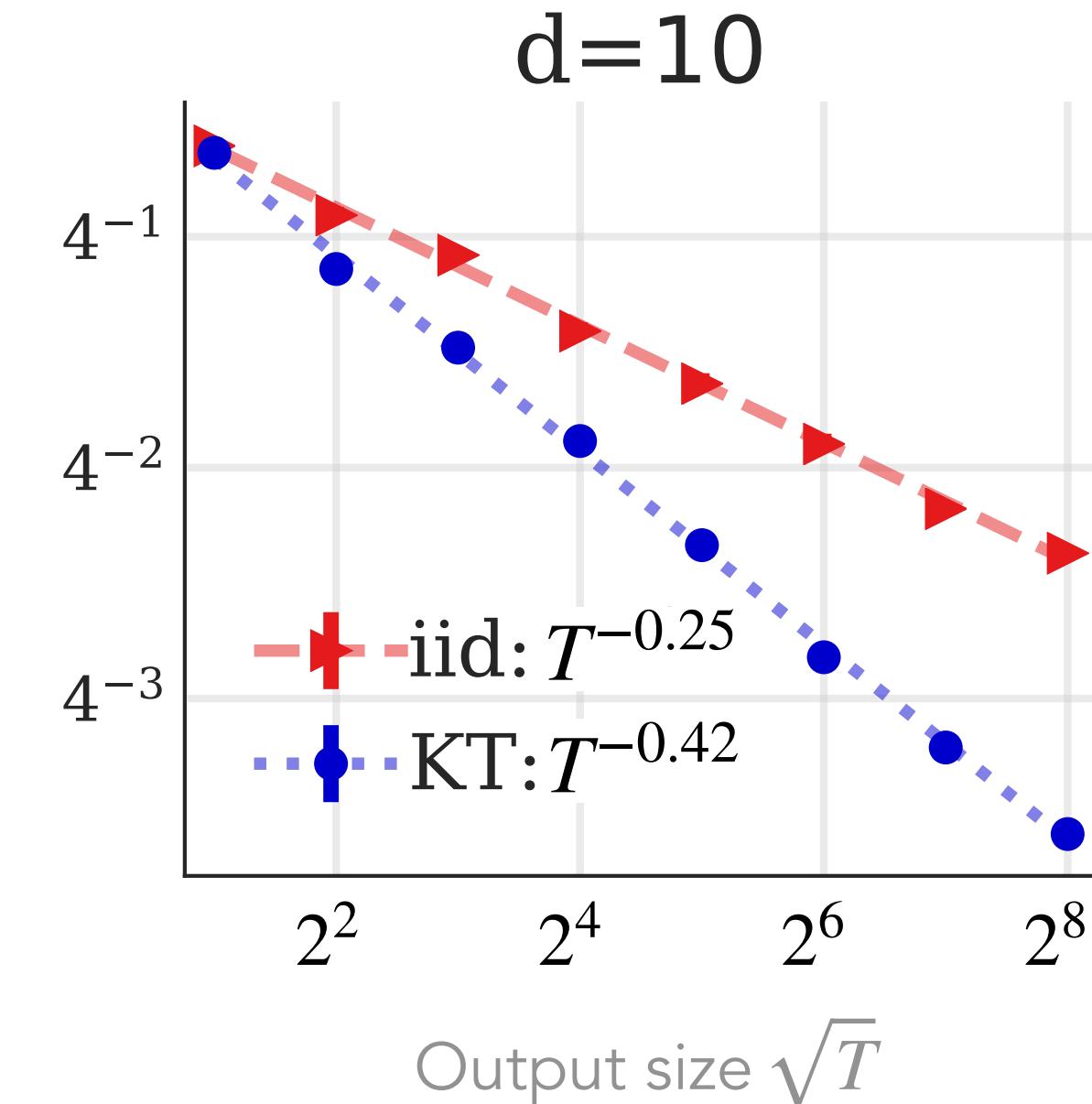
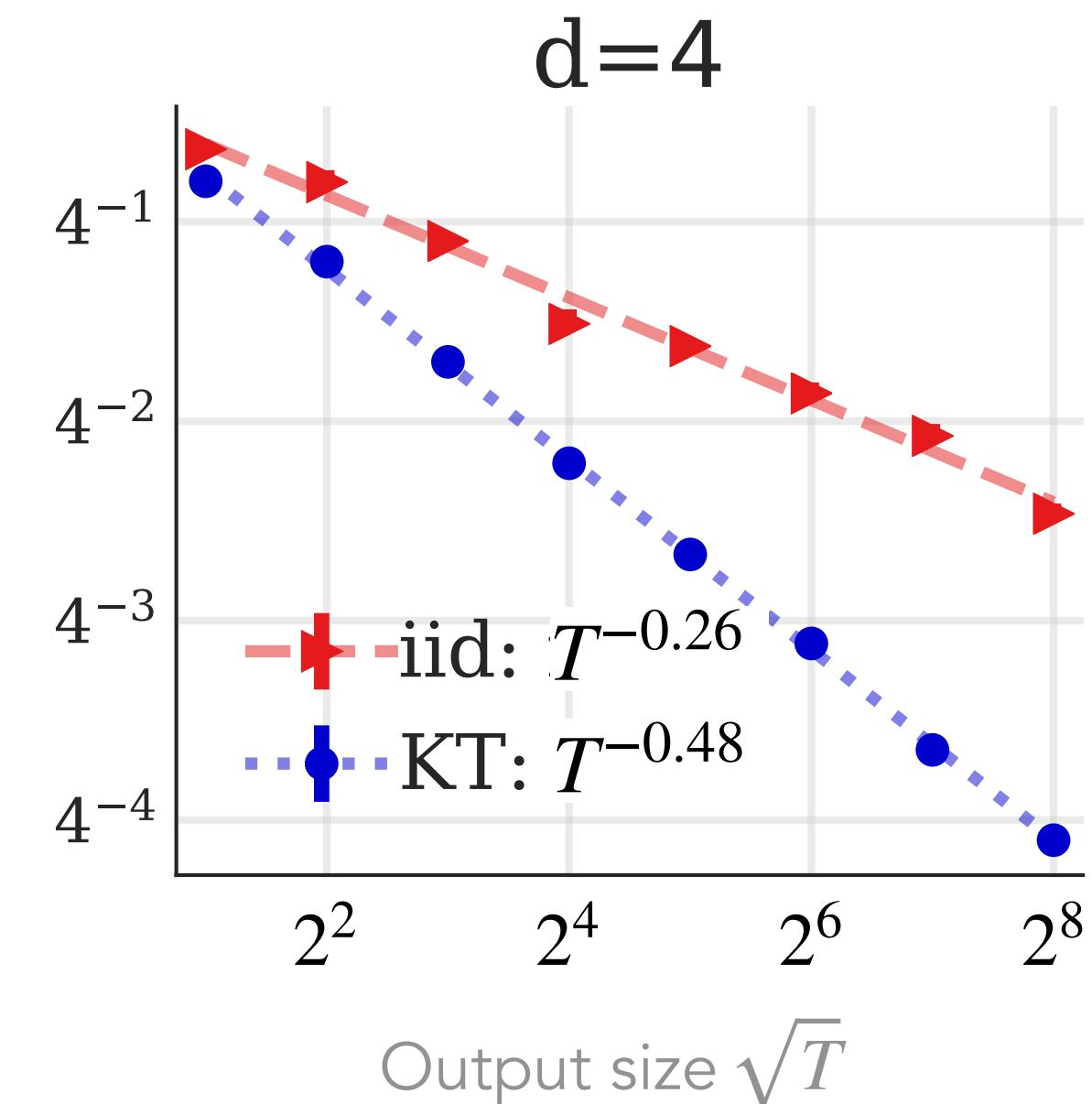
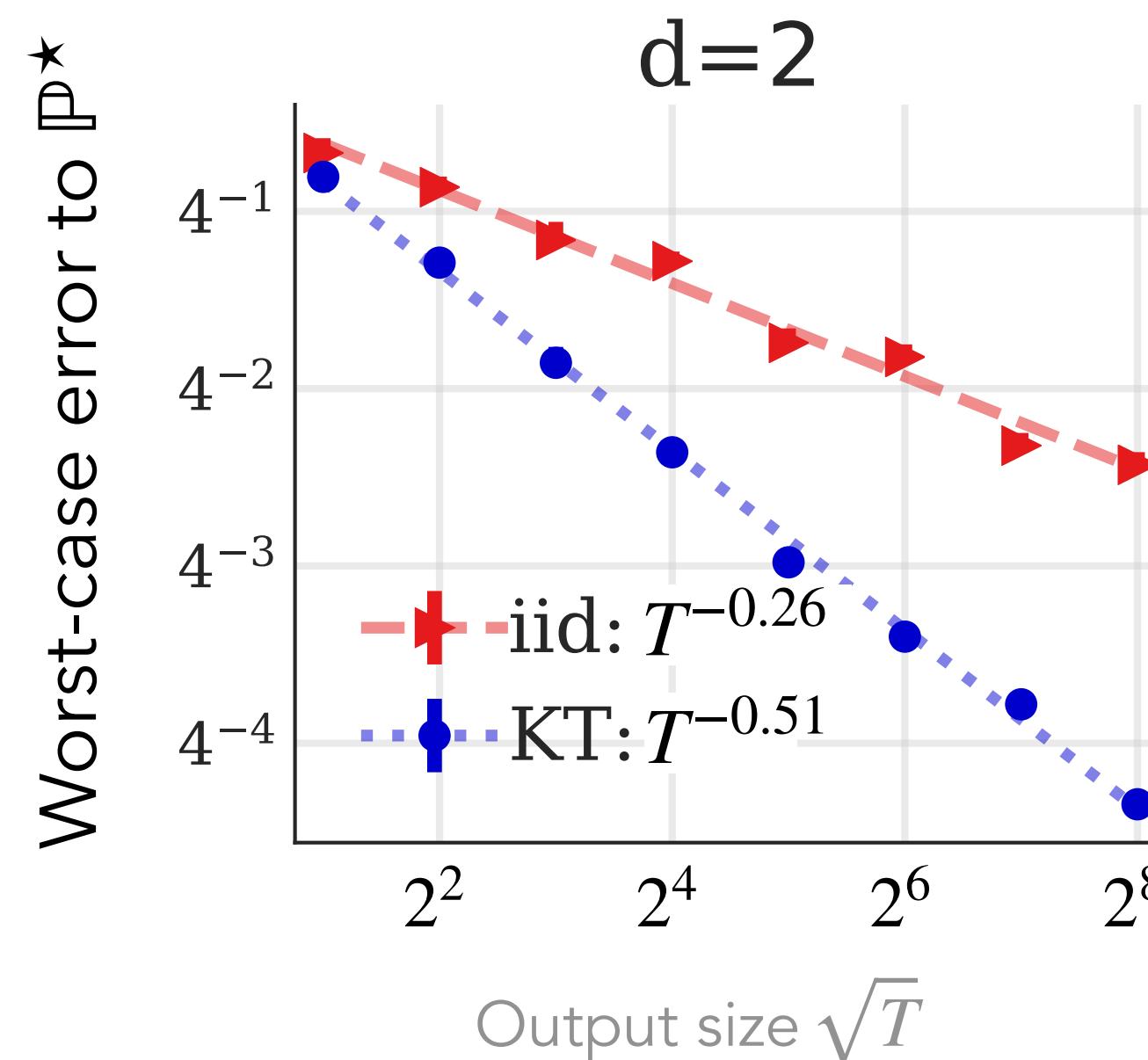
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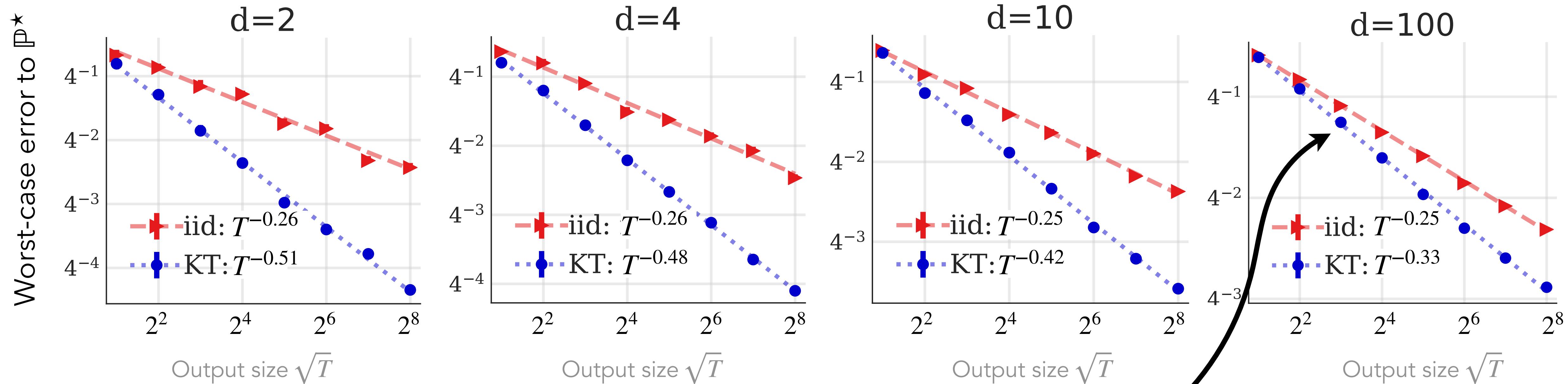
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**Significant gains in $d = 100$
with just 8 output points**

KT on MCMC points for \mathbb{P}^* in experiments ($d = 38$)

[†]Input = 2 MCMC runs on 2 posteriors \mathbb{P}^* , Gaussian kernel

Worst-case error to \mathbb{P}_T

[[†]MCMC data from Riabiz-Chen-Cockayne-Swietach-Niederer-Mackey-Oates '21]

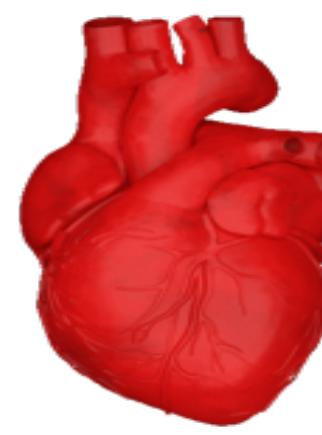
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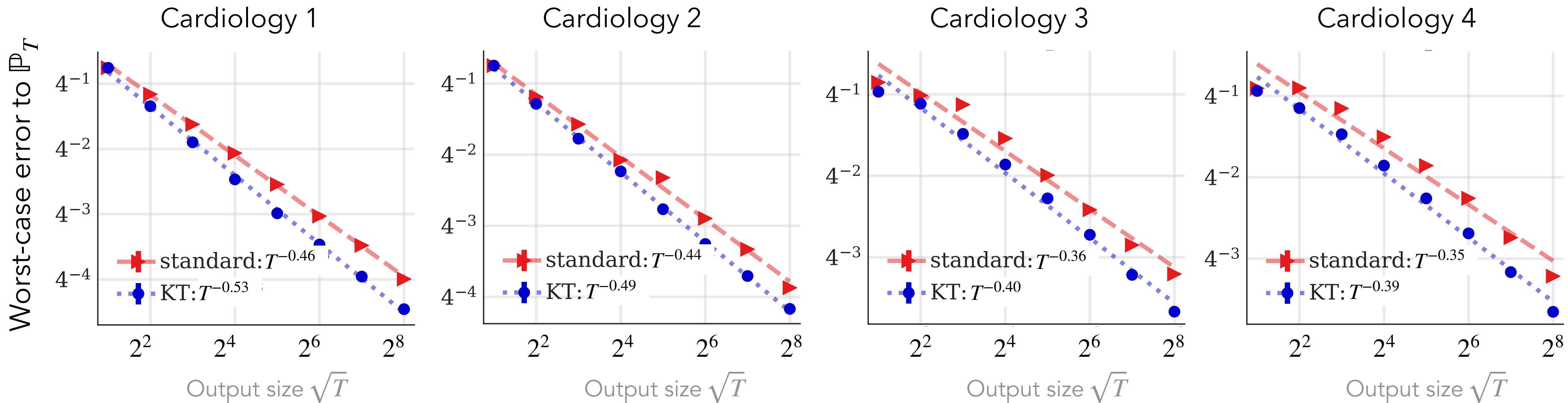
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KT on MCMC points for \mathbb{P}^* in experiments ($d = 38$)



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Standard thinning does well but **KT provides further improvement**
& offers **50% computational savings** (each point ~ 4 CPU weeks)

[[†]MCMC data from Riabiz-Chen-Cockayne-Swietach-Niederer-Mackey-Oates '21]

Kernel thinning: Near-optimal compression in near-linear time

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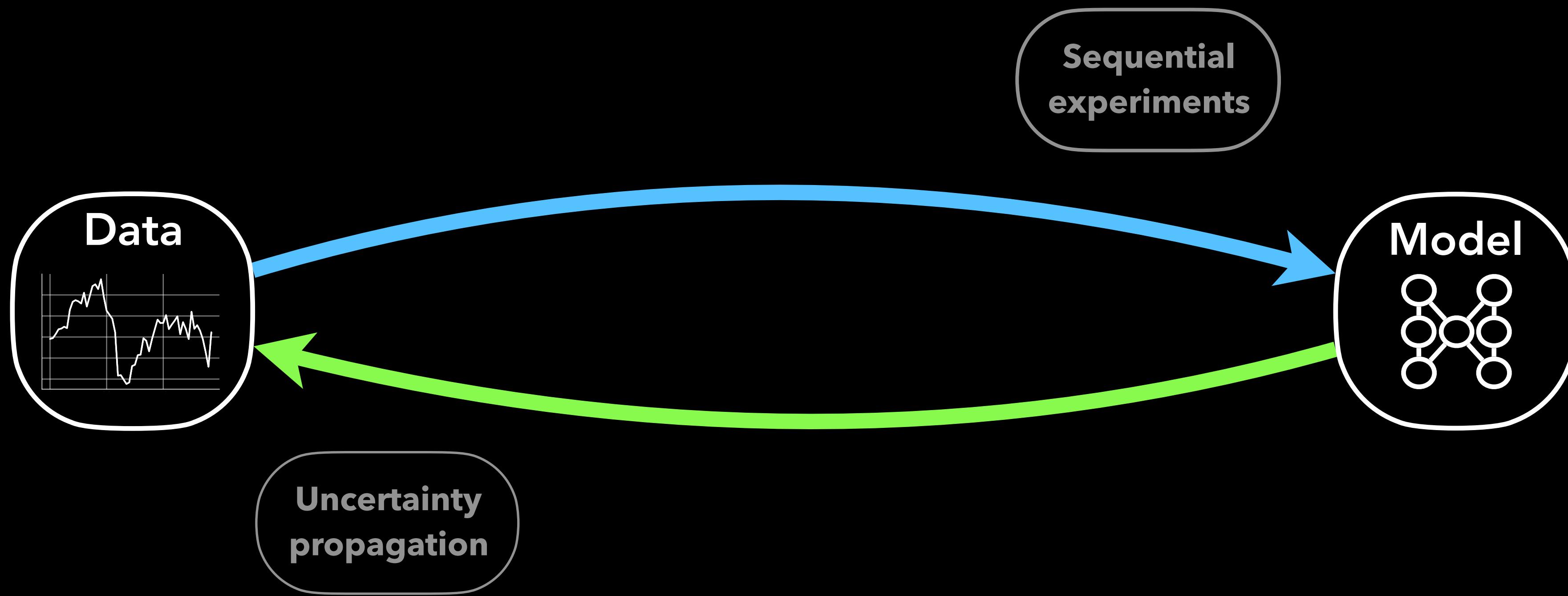


python™

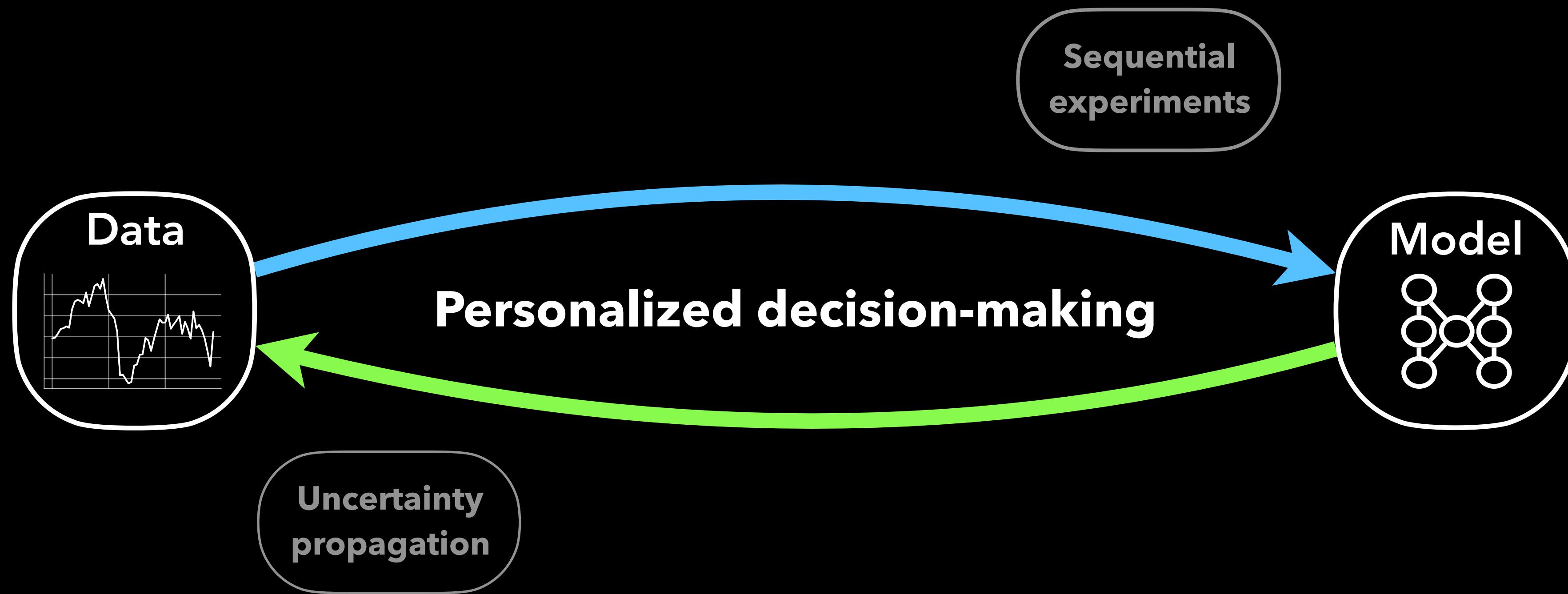
pip install goodpoints

Thin 100k points in 100 dimensions in 10mins

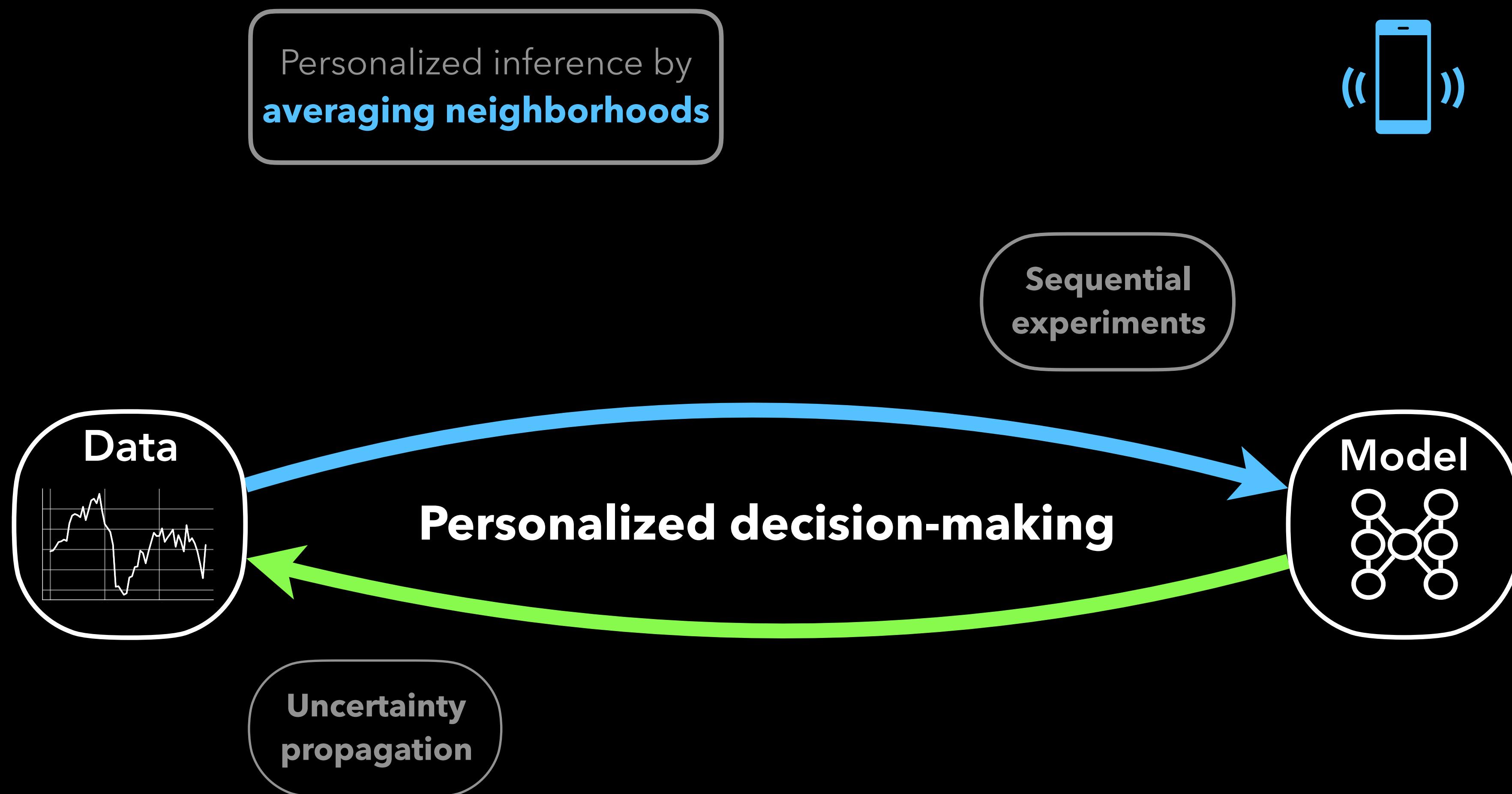
talk summary



talk summary

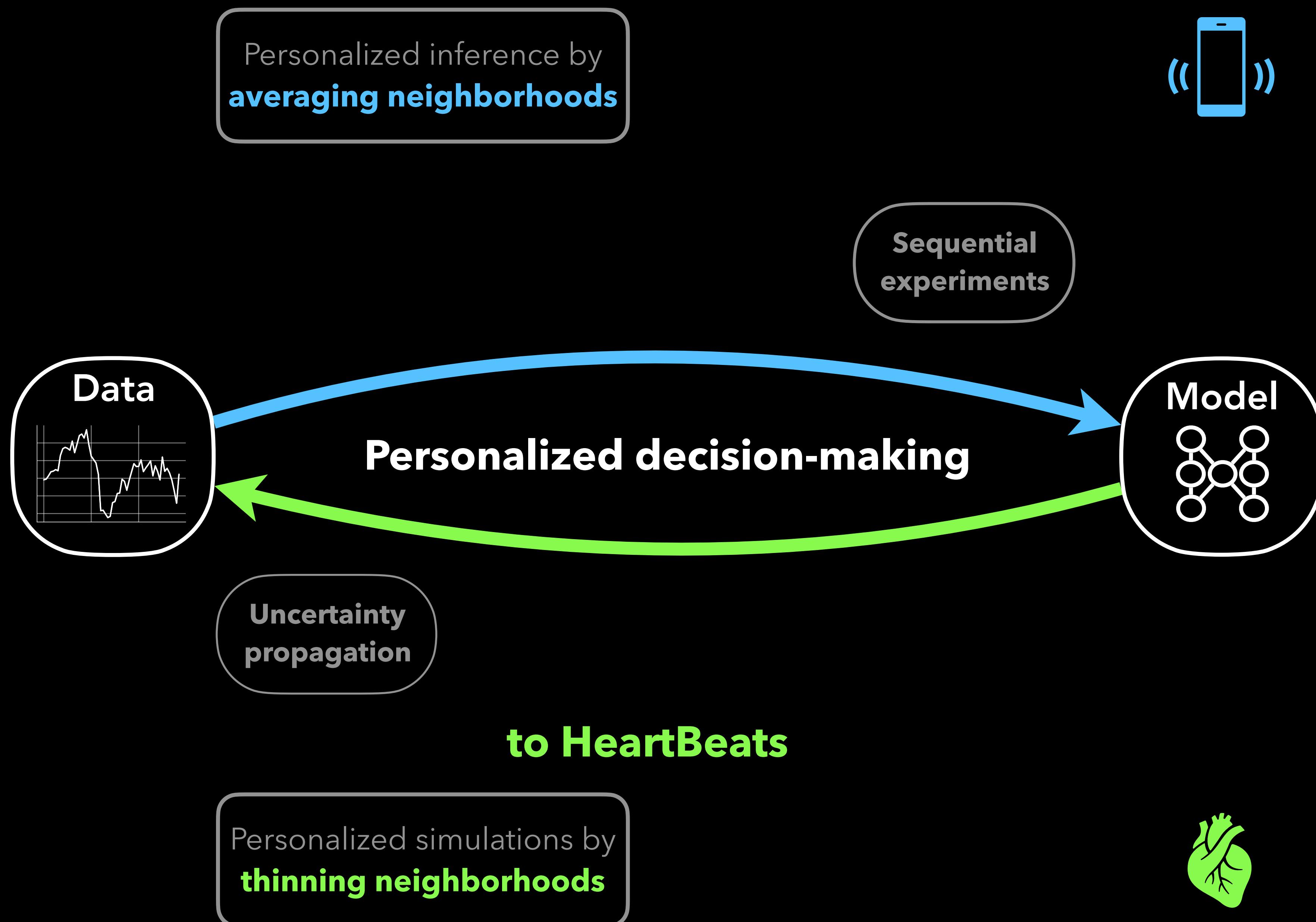


From HeartSteps



talk summary

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talk summary

From HeartSteps

Personalized inference by
averaging neighborhoods

**Quadratic gains via
double robustness**



Sequential
experiments



to HeartBeats

Personalized simulations by
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talk summary

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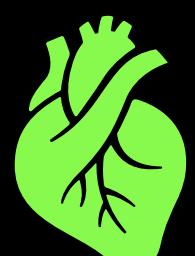
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to HeartBeats

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to HeartBeats

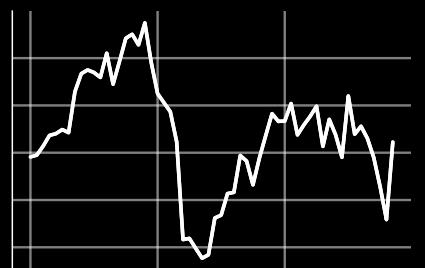
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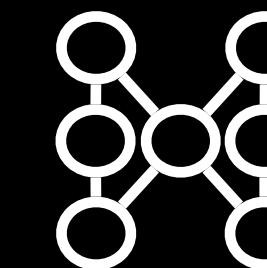


**Sequential
experiments**

Data



Model



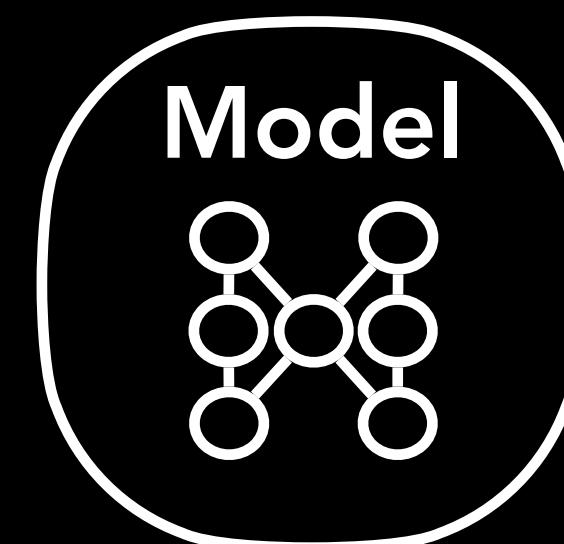
**Uncertainty
propagation**



Uncertainty
propagation

Data and computation efficient methods for personalized decision-making

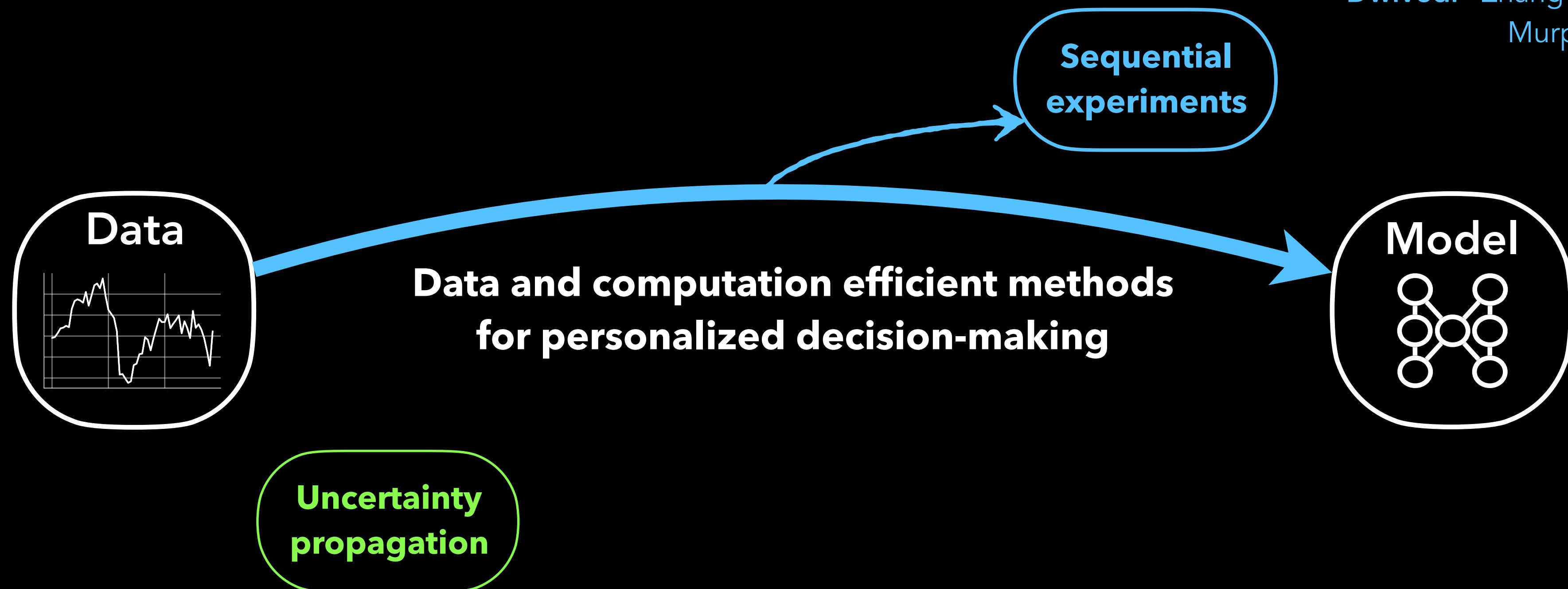
Sequential
experiments



Deep dive into personalization by a reinforcement learning algorithm

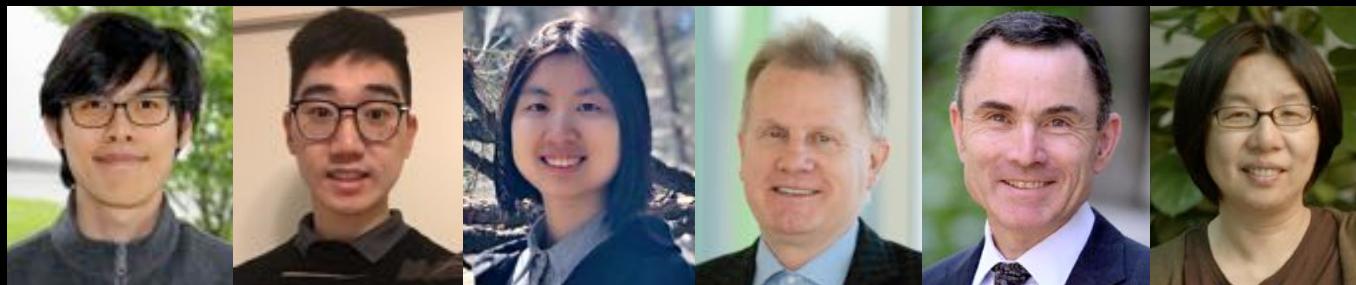


Dwivedi*-Zhang*-Chhabria-Klasnja-Murphy '23



research overview

Stable discovery of interpretable subgroups in randomized studies via calibration

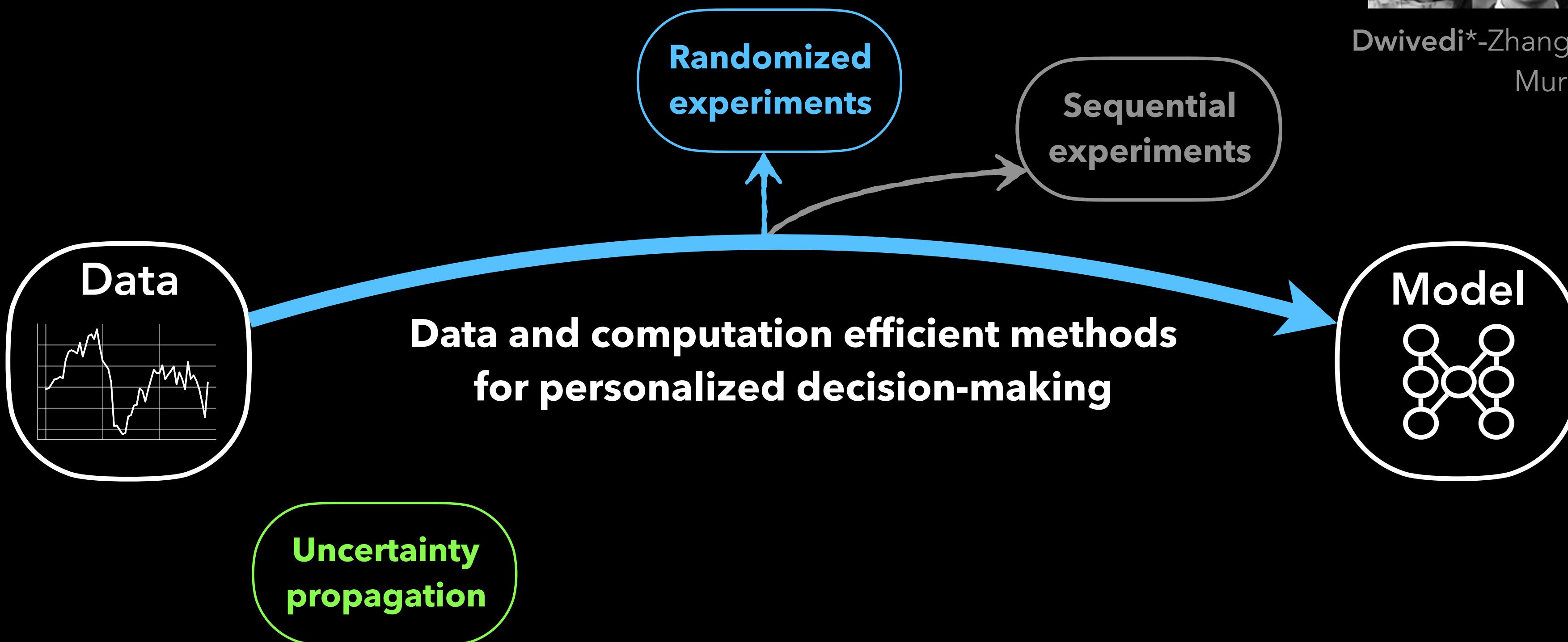


Dwivedi*-Tan*-Park-Wei-Horgan-Madigan-Yu '20

Deep dive into personalization by a reinforcement learning algorithm



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research overview

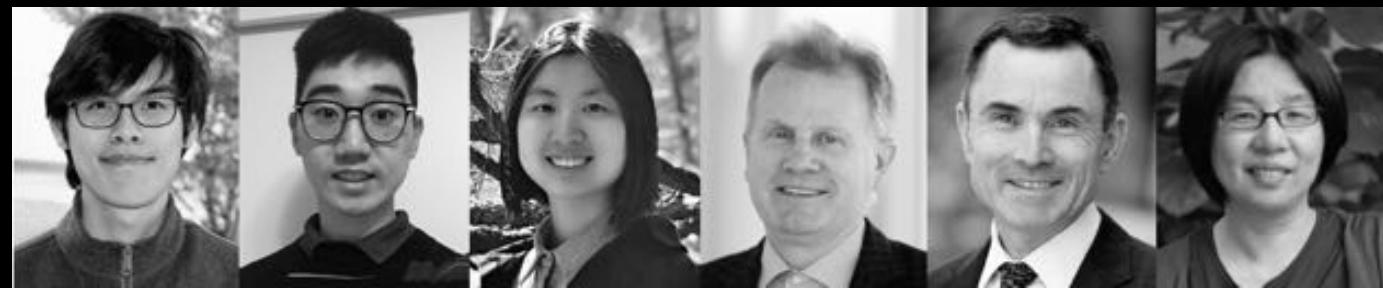
Stable discovery of interpretable subgroups in randomized studies via calibration



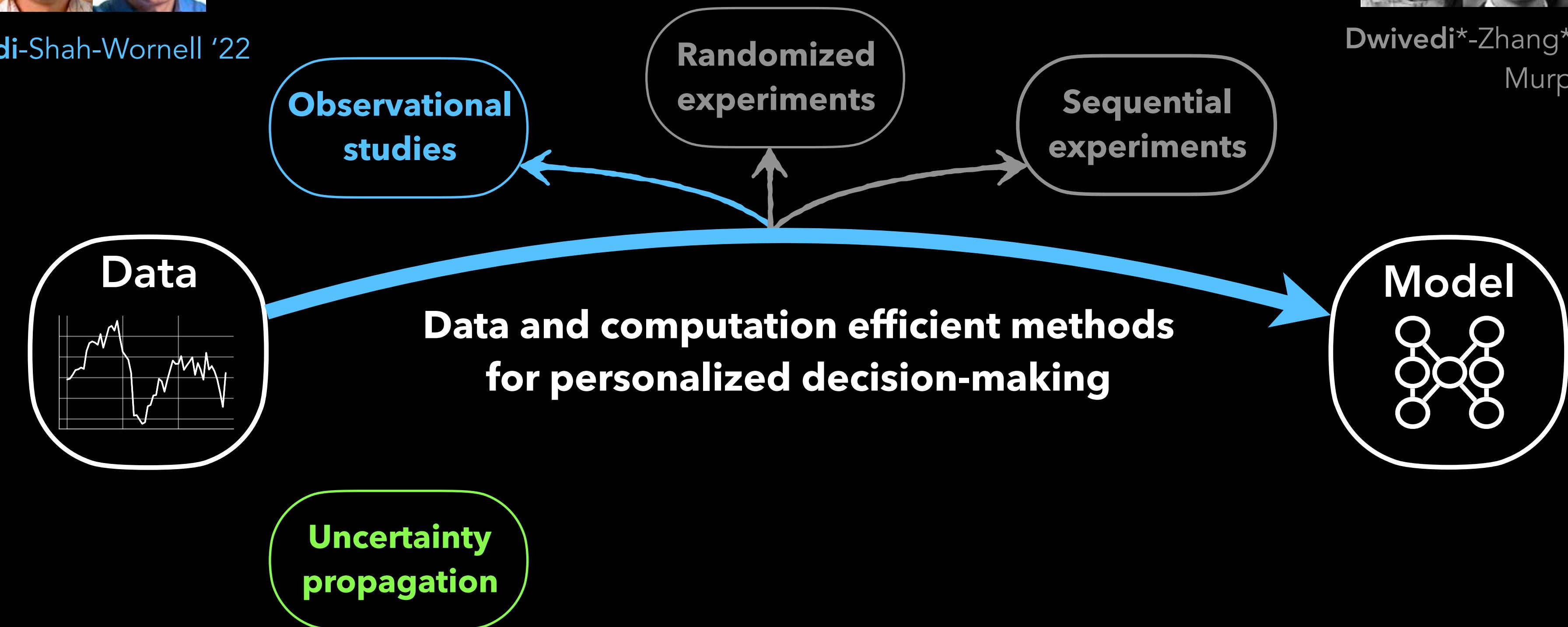
On counterfactual inference with unobserved confounding via exponential family



Shah-Dwivedi-Shah-Wornell '22



Dwivedi*-Tan*-Park-Wei-Horgan-Madigan-Yu '20



Deep dive into personalization by a reinforcement learning algorithm



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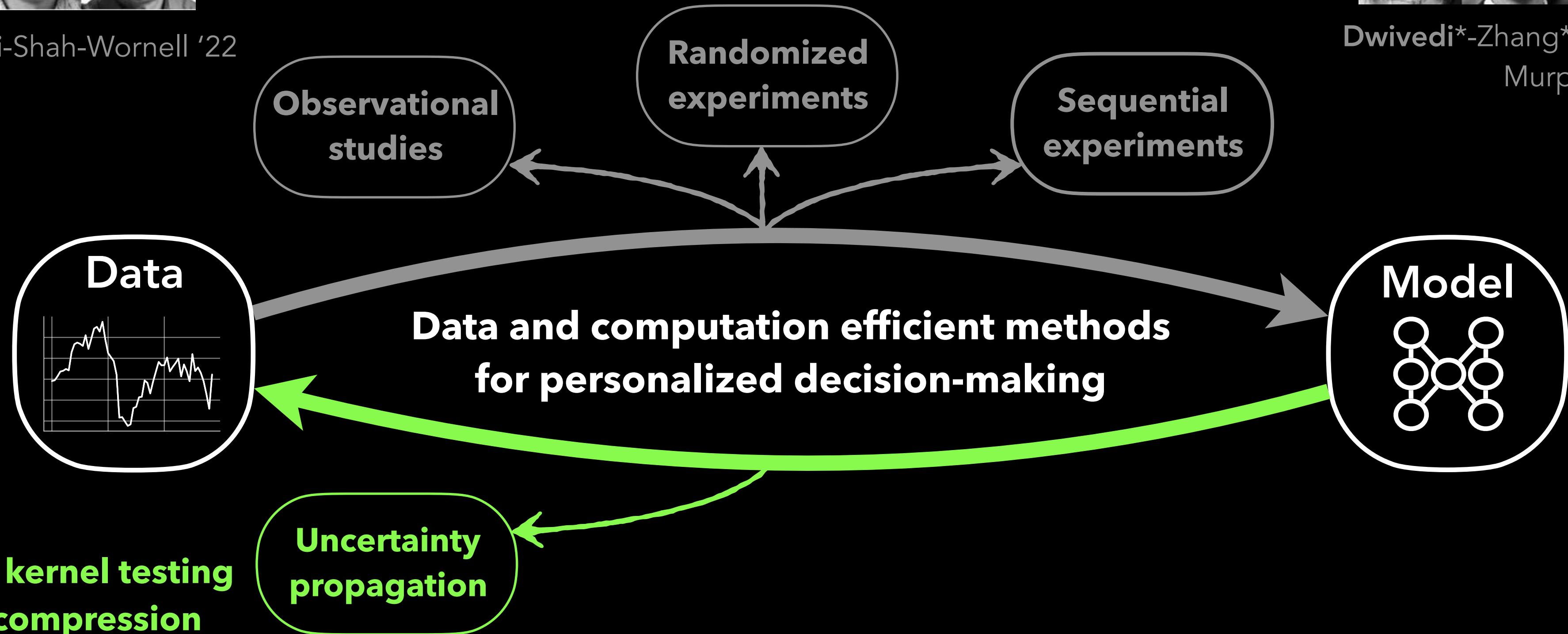


Dwivedi*-Tan*-Park-Wei-Horgan-Madigan-Yu '20

Deep dive into personalization by a reinforcement learning algorithm



Dwivedi*-Zhang*-Chhabria-Klasnja-Murphy '23



Fast and powerful kernel testing via distribution compression



Shetty-Dwivedi-Mackey '22,
Domingo Enrich-Dwivedi-Mackey '23

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Shah-Dwivedi-Shah-Wornell '22

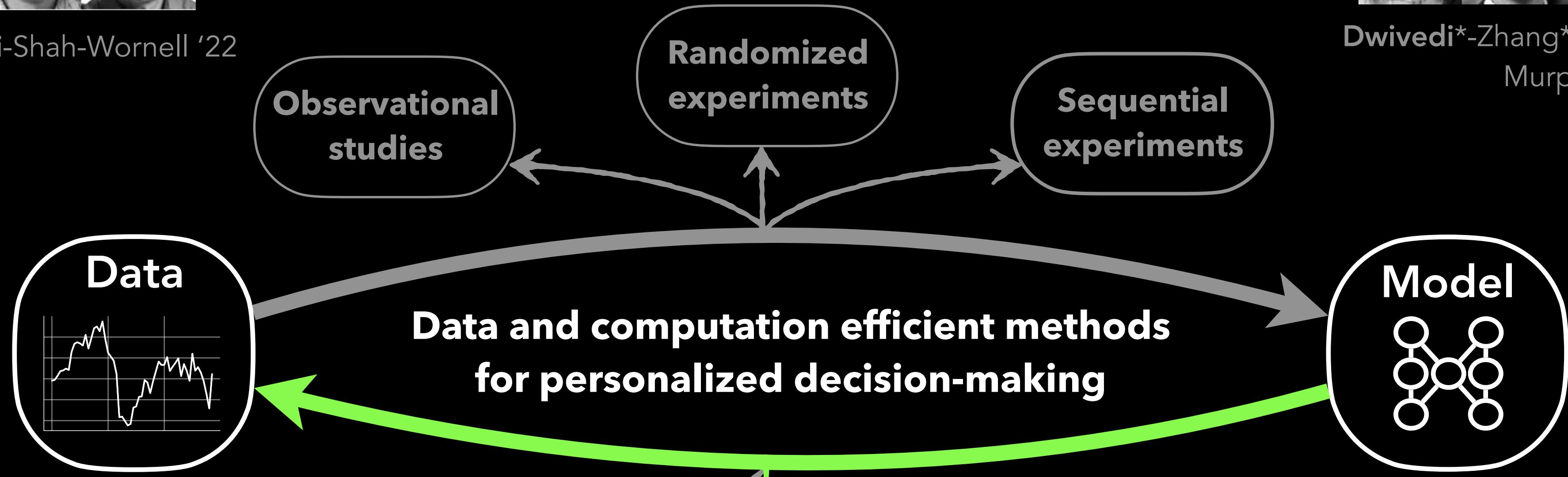


Dwivedi*-Tan*-Park-Wei-Horgan-Madigan-Yu '20

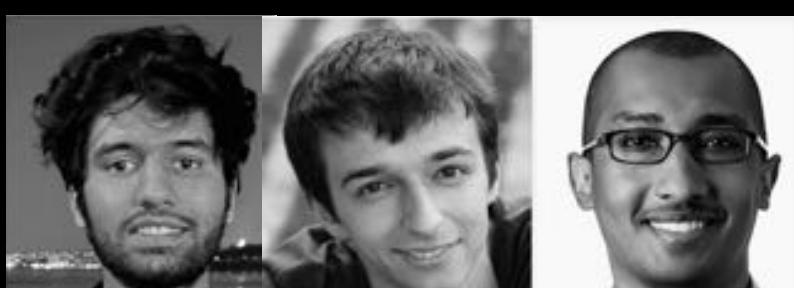
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Mixing time guarantees for MCMC algorithms in high dimensions



Chen*-Dwivedi*-Wainwright-Yu '18, '19, '20

research overview

Stable discovery of interpretable subgroups in randomized studies via calibration



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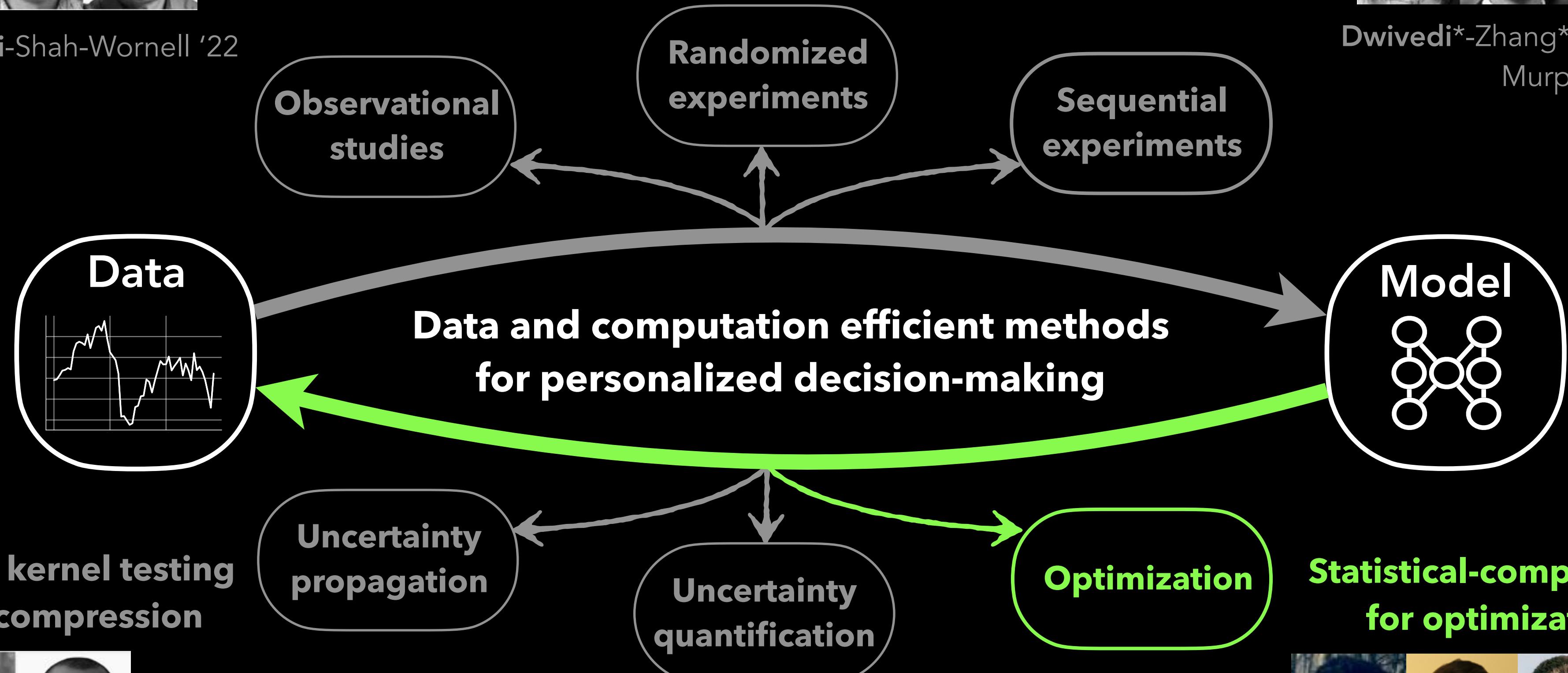


Dwivedi*-Tan*-Park-Wei-Horgan-Madigan-Yu '20

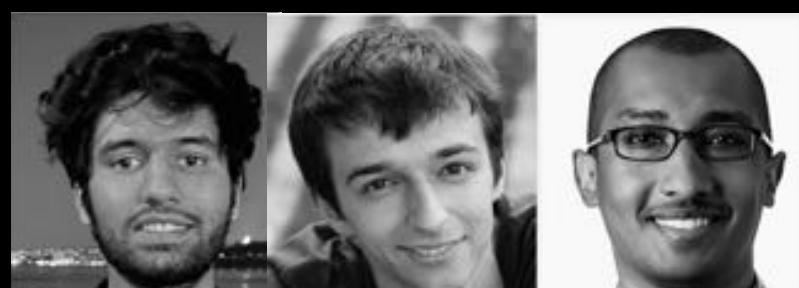
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Chen*-Dwivedi*-Wainwright-Yu '18, '19, '20

Statistical-computational tradeoffs for optimization algorithms



Dwivedi*-Ho*-Khamaru*-Wainwright-Jordan-Yu '19, '20, '21, '22+

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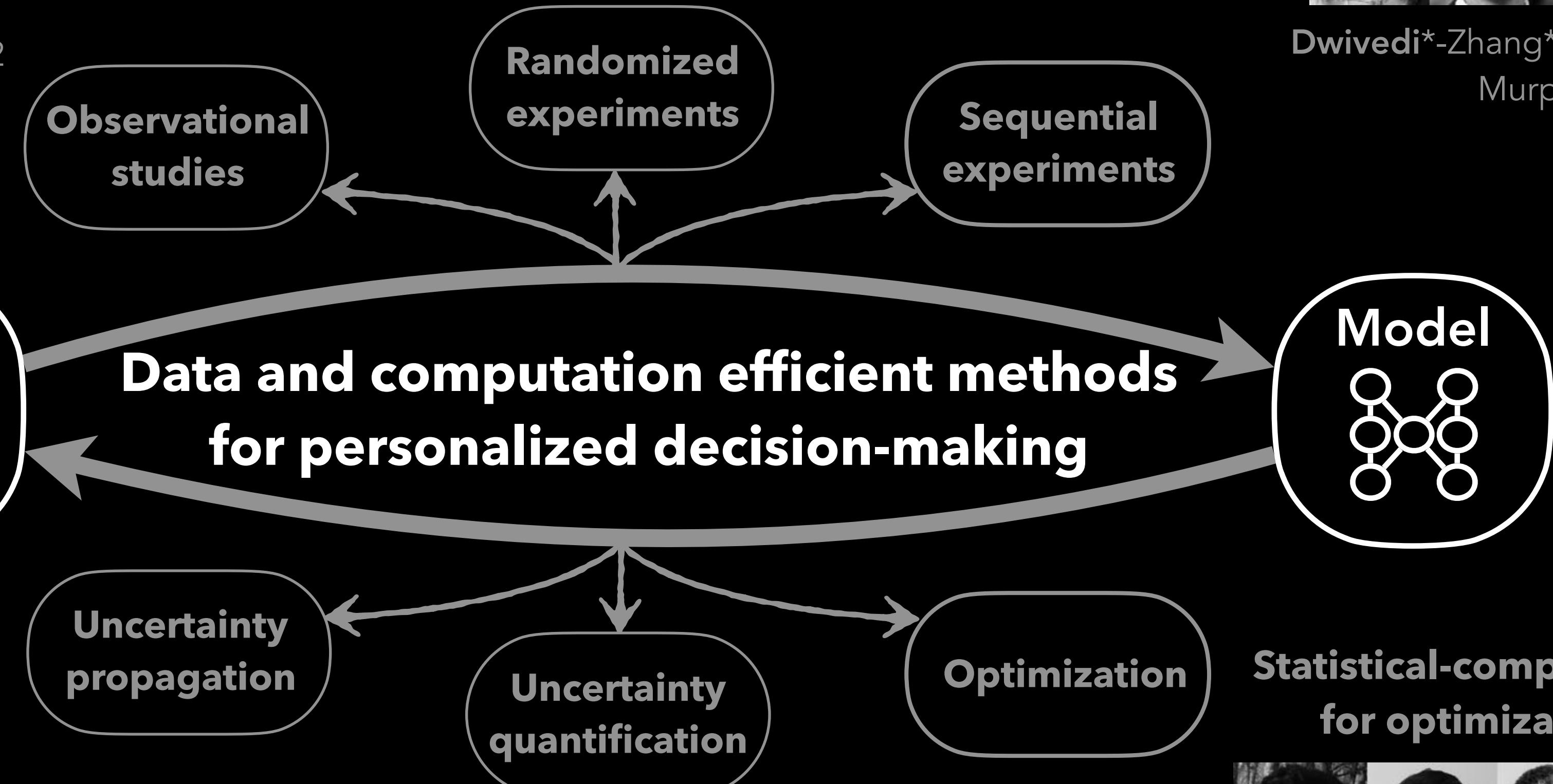


Dwivedi*-Tan*-Park-Wei-Horgan-Madigan-Yu '20

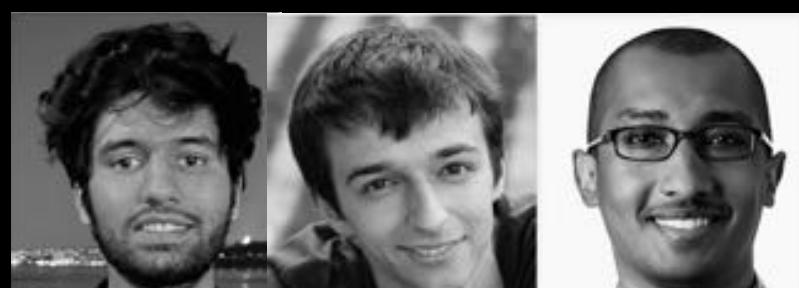
Deep dive into personalization by a reinforcement learning algorithm



Dwivedi*-Zhang*-Chhabria-Klasnja-Murphy '23



Fast and powerful kernel testing via distribution compression



Shetty-Dwivedi-Mackey '22,
Domingo Enrich-Dwivedi-Mackey '22

Mixing time guarantees for MCMC algorithms in high dimensions



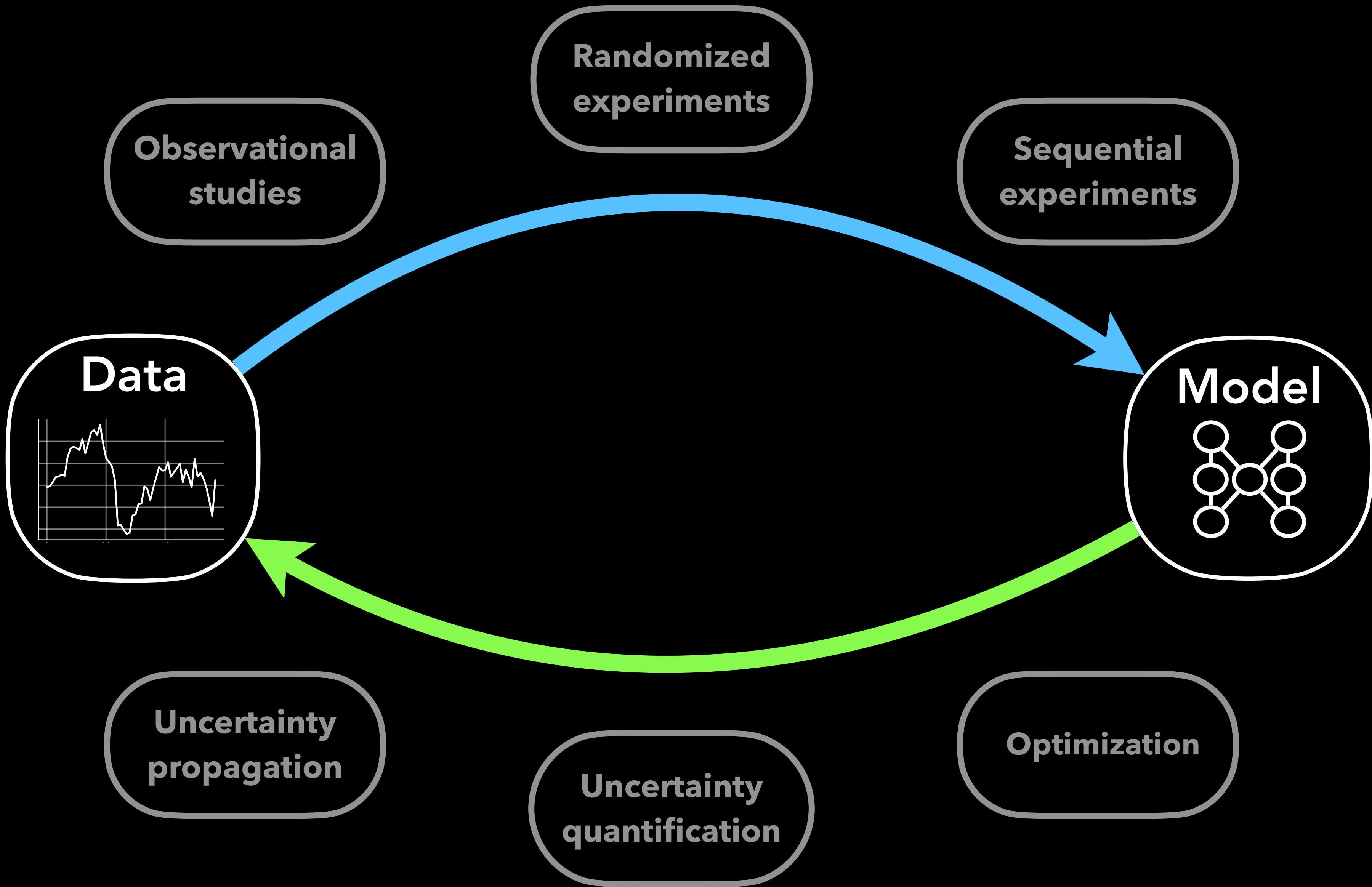
Chen*-Dwivedi*-Wainwright-Yu '18, '19, '20

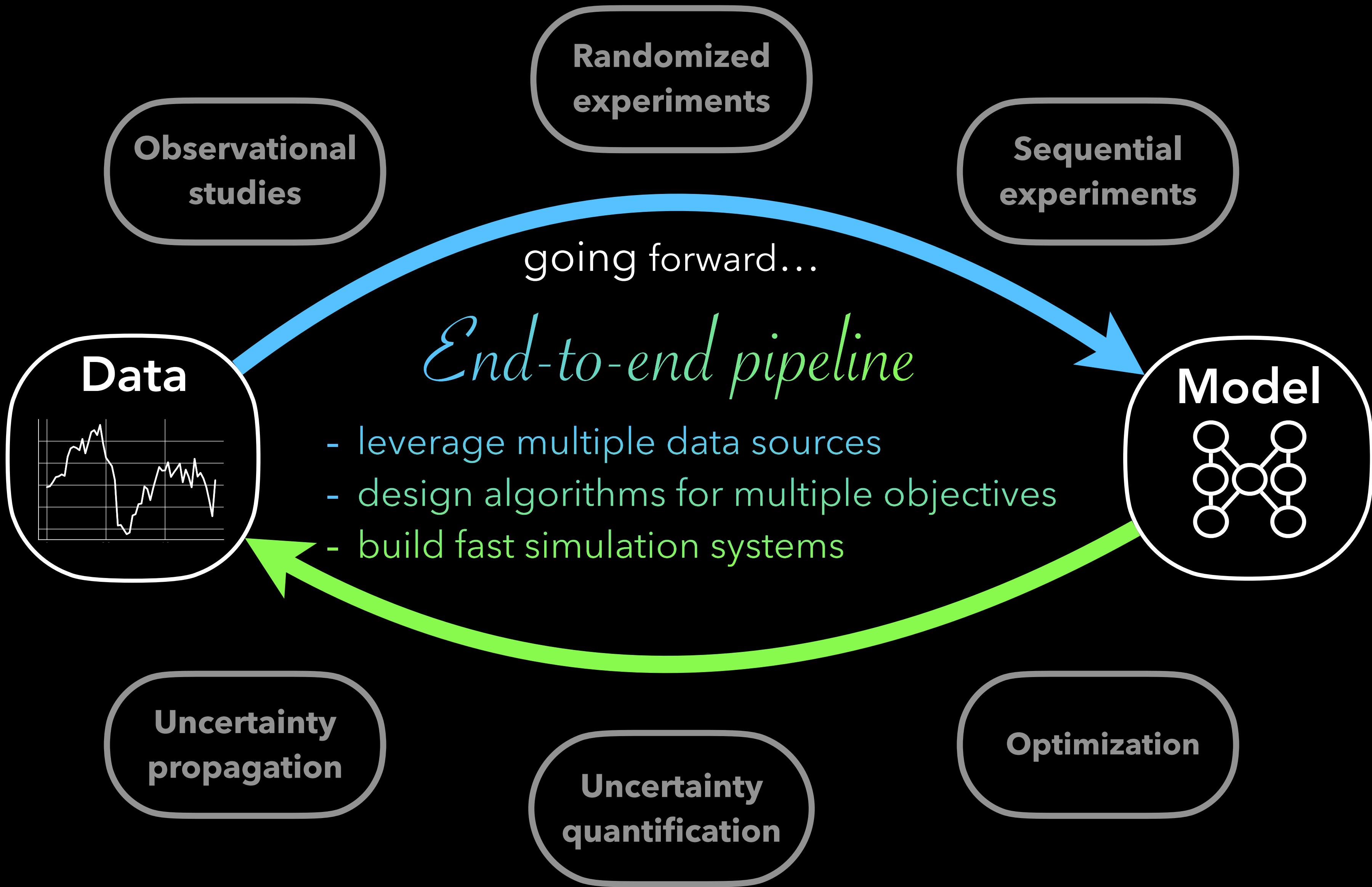
Statistical-computational tradeoffs for optimization algorithms



Dwivedi*-Ho*-Khamaru*-Wainwright-Jordan-Yu '19, '20, '21, '22+

research overview





Thank you!

raazdwivedi.github.io