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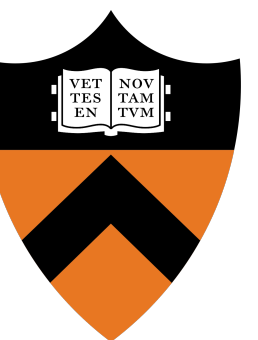
# Accelerating system simulation, identification and design with ML

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Alex Beatson

Princeton University  
Department of Computer Science

In collaboration with: Ryan P. Adams, Jordan Ash, Geoffrey Roeder, Tianju Xie

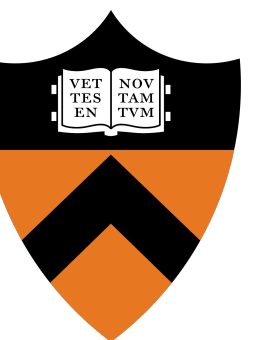


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# SIMULATION AND NUMERICAL METHODS

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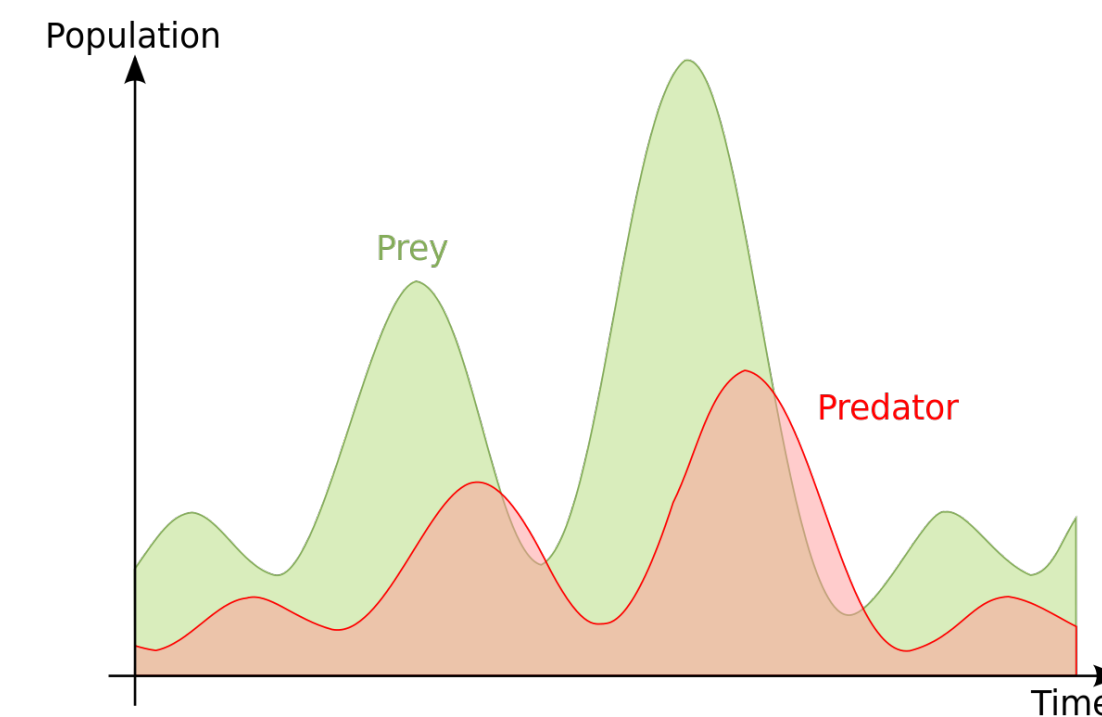
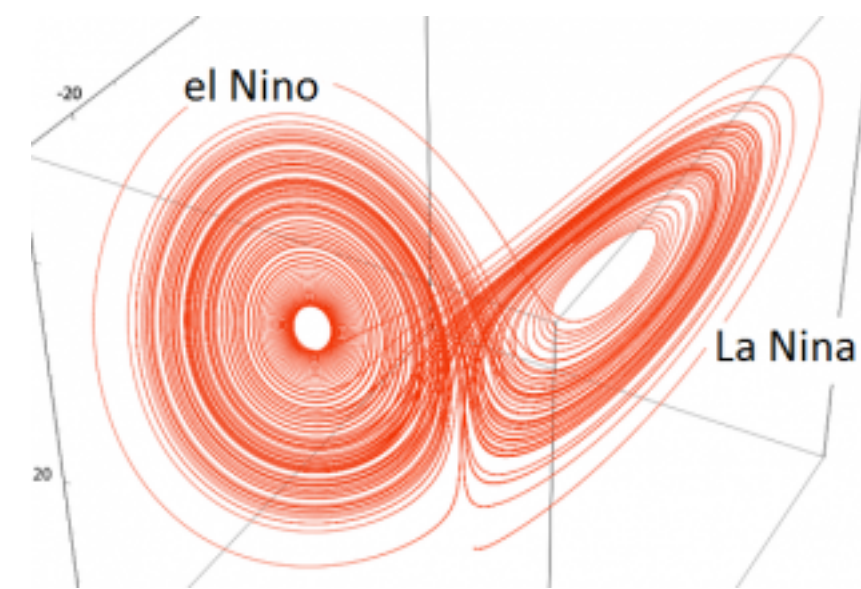
Numerical methods enable model-based reasoning about the world.



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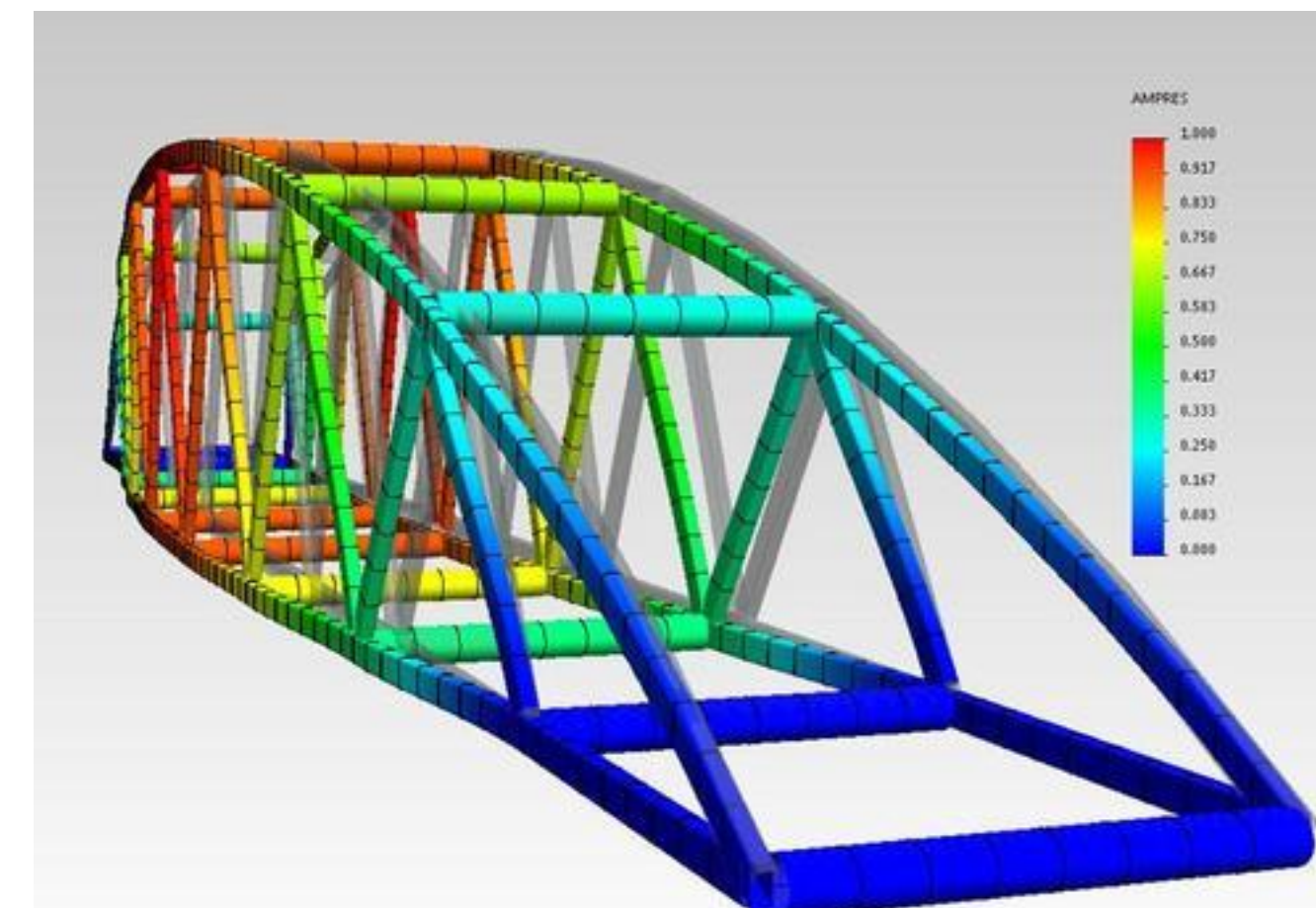
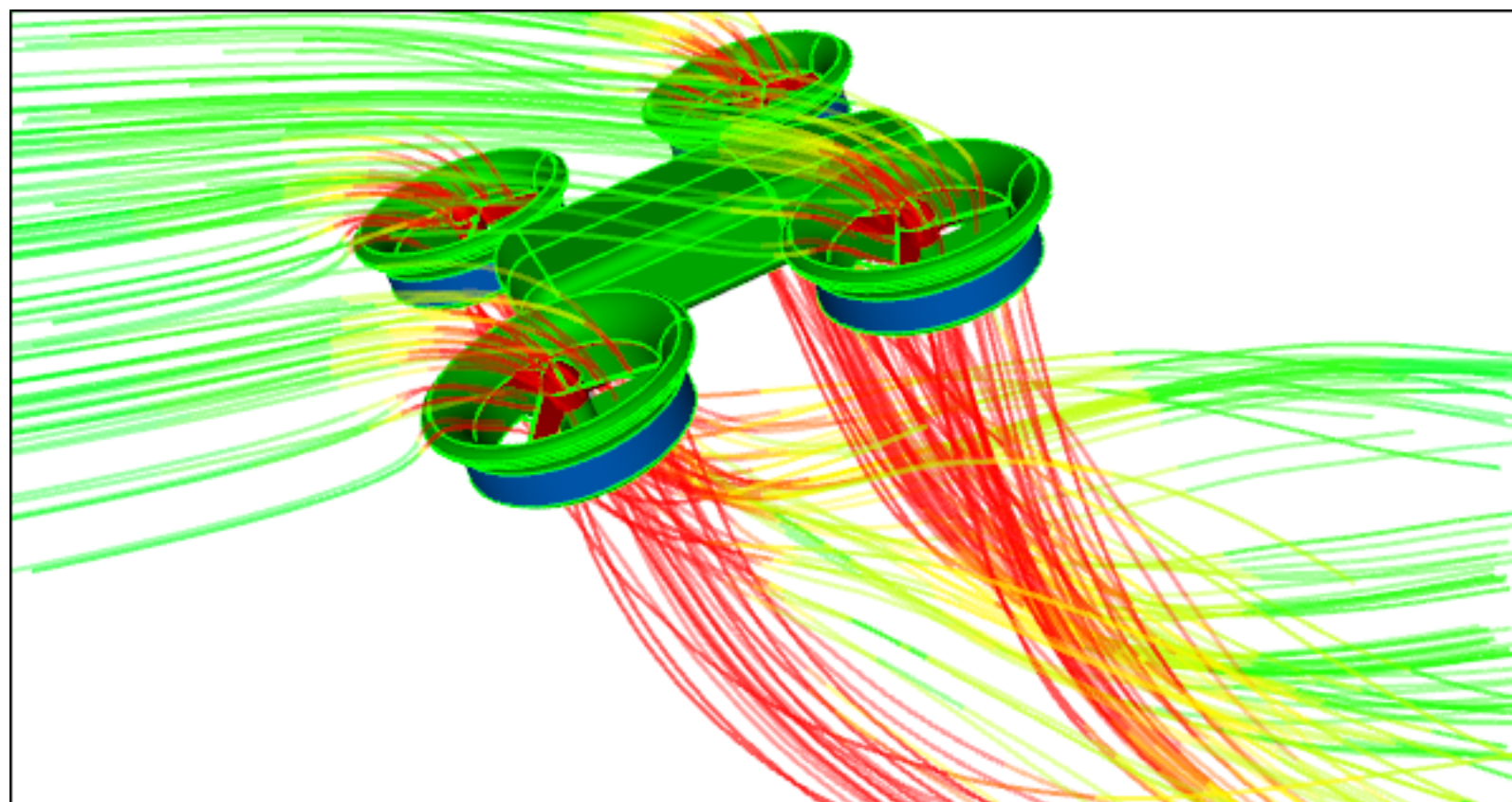
e.g. ODEs (solved with Euler, Runge-Kutta, ...)



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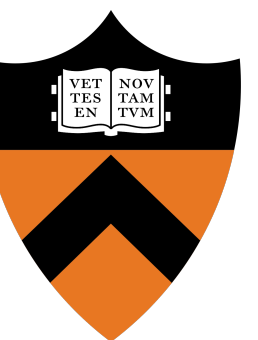
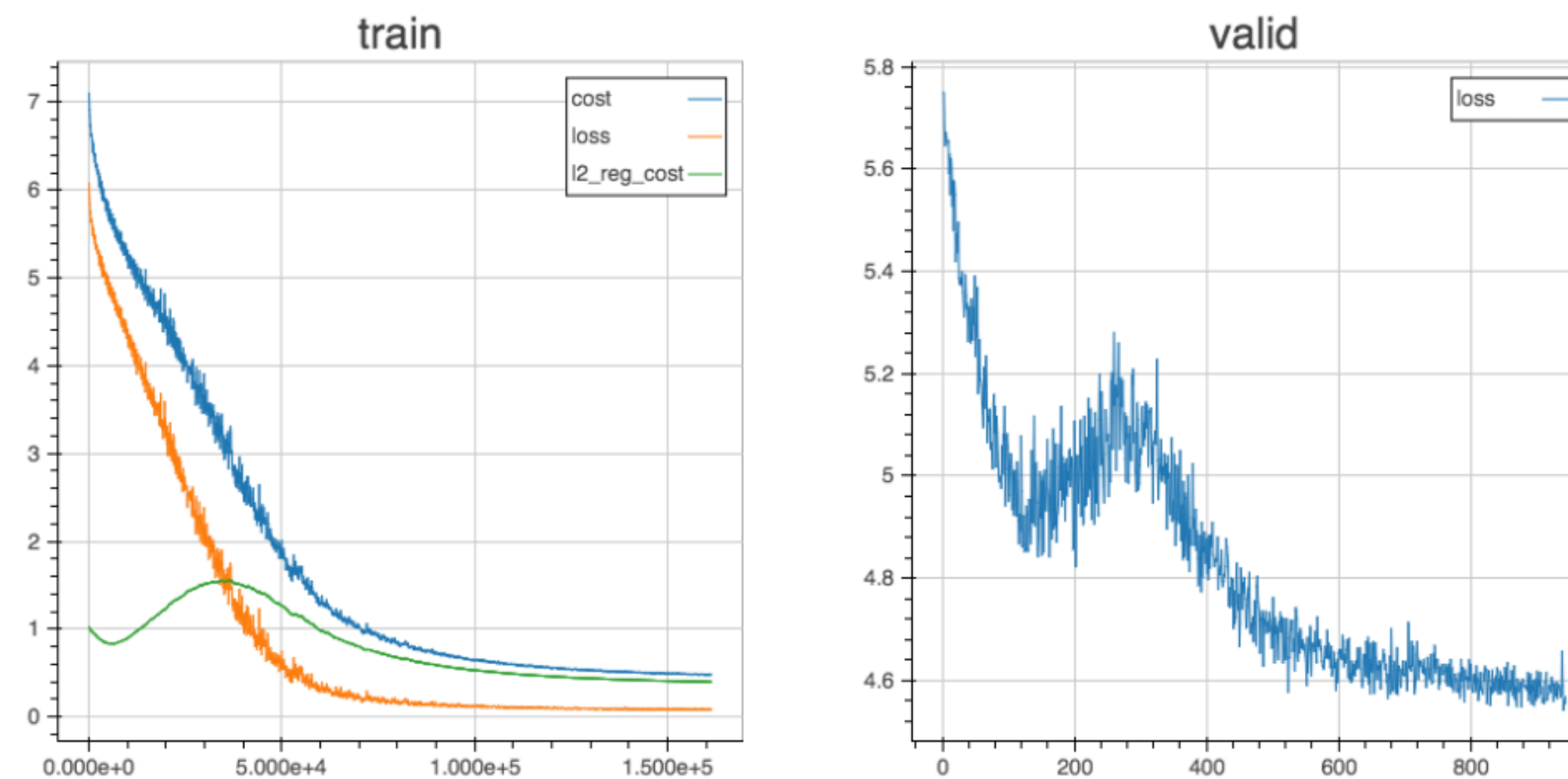
e.g. PDEs (solved with Finite Element Analysis, Finite Volume Method, ...)



# SIMULATION AND NUMERICAL METHODS

Numerical methods enable model-based reasoning about the world.

e.g. evaluating ML algorithms / architectures by training with SGD





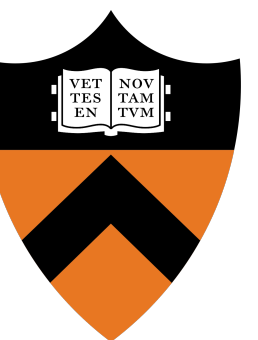
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# MODEL-BASED OPTIMIZATION

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Numerical methods enable model-based reasoning about the world.

Optimizing the output of a numerical method with respect to system parameters allows system identification, design, and control.

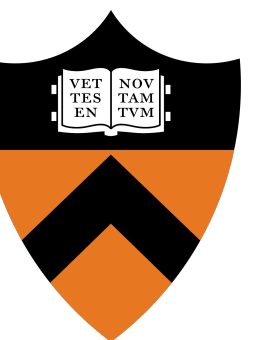


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# BOTTLENECKS

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- Model design and parametrization
- Numerical method implementation and tuning
- Computation

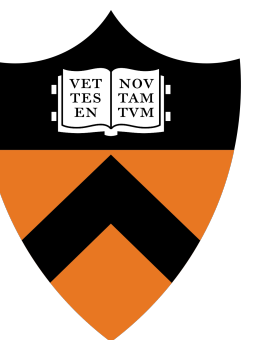


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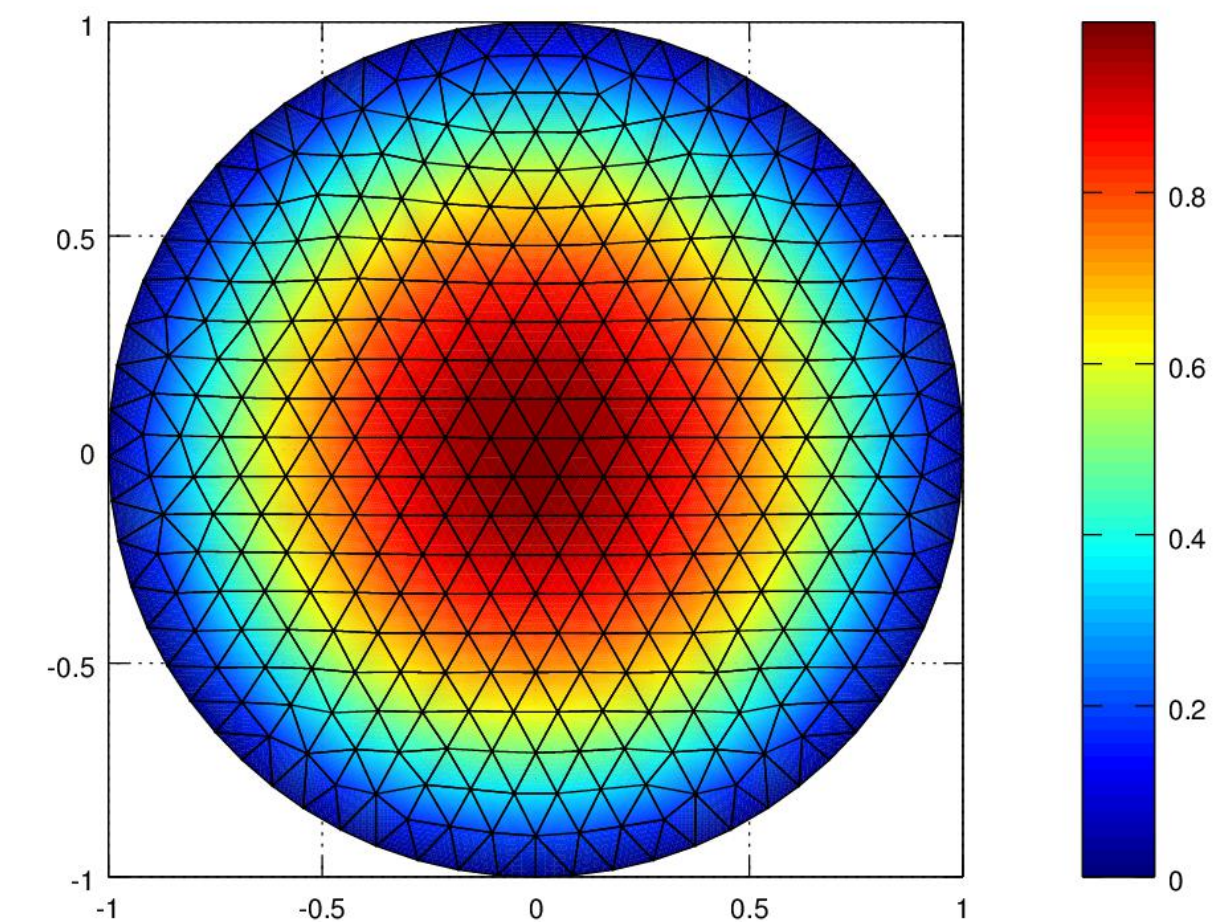
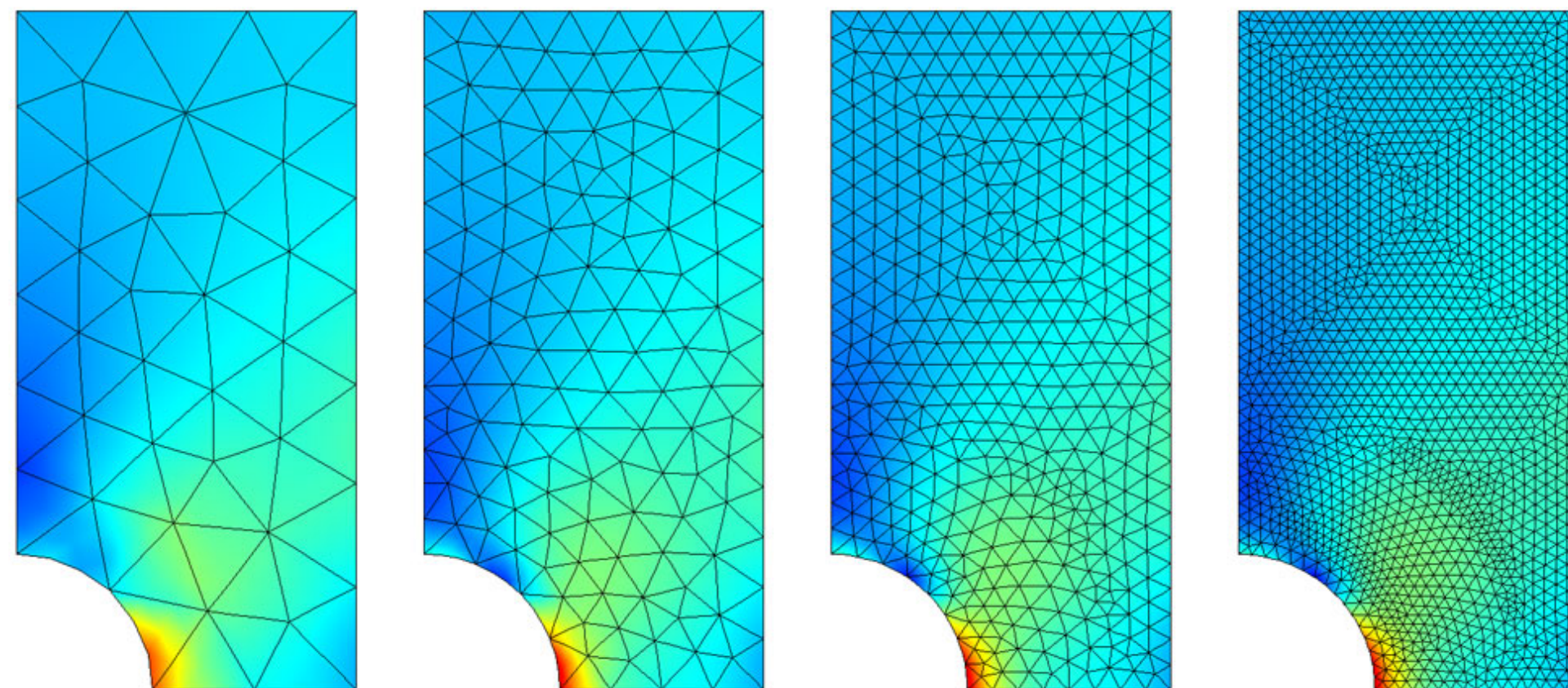
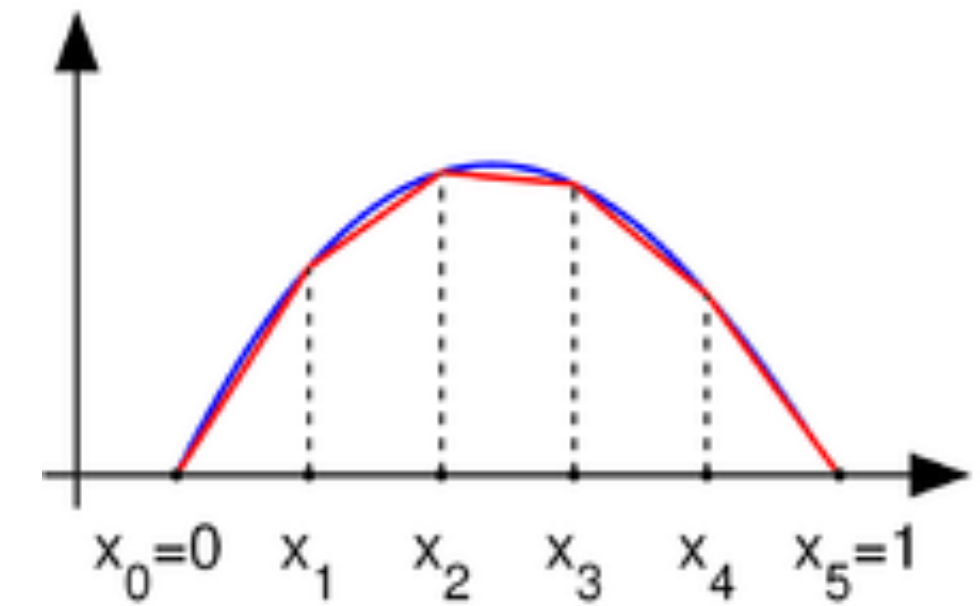




# COMMON STRUCTURE

Discretization through time, space, or iterations

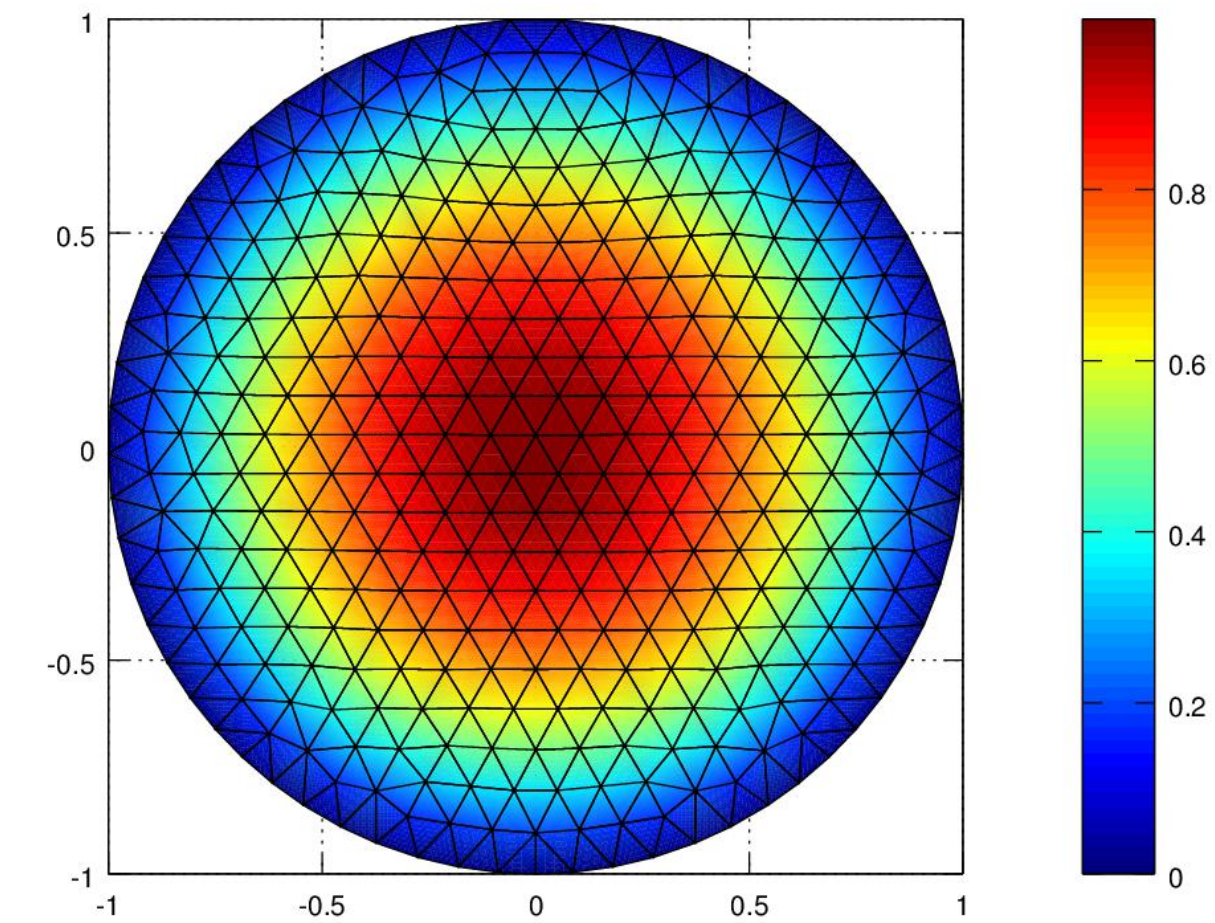
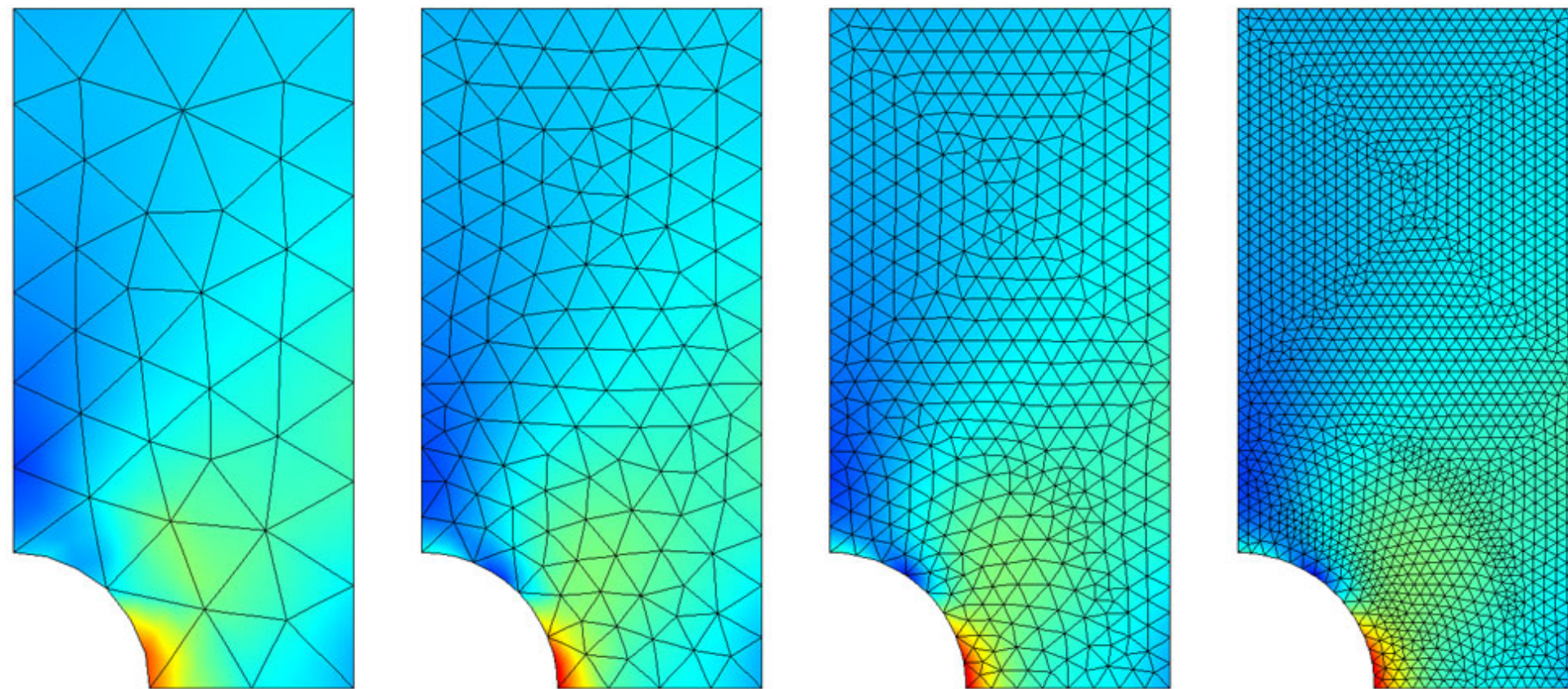
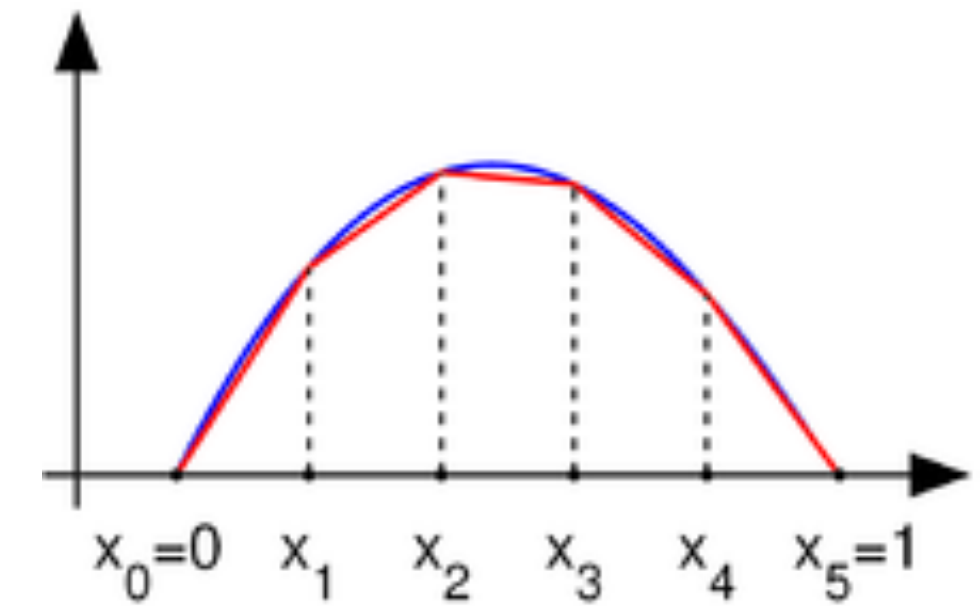
Increasing accuracy with increasing computation





# GOAL

Develop ML tools which exploit this structure to accelerate system simulation, identification, and design.



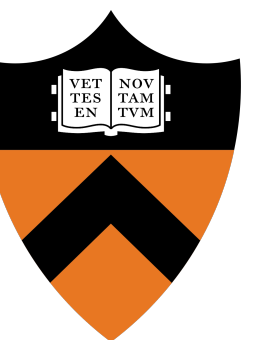
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# Efficient Optimization of Loops and Limits with Randomized Telescoping Sums

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with Ryan P. Adams

ICML 2019

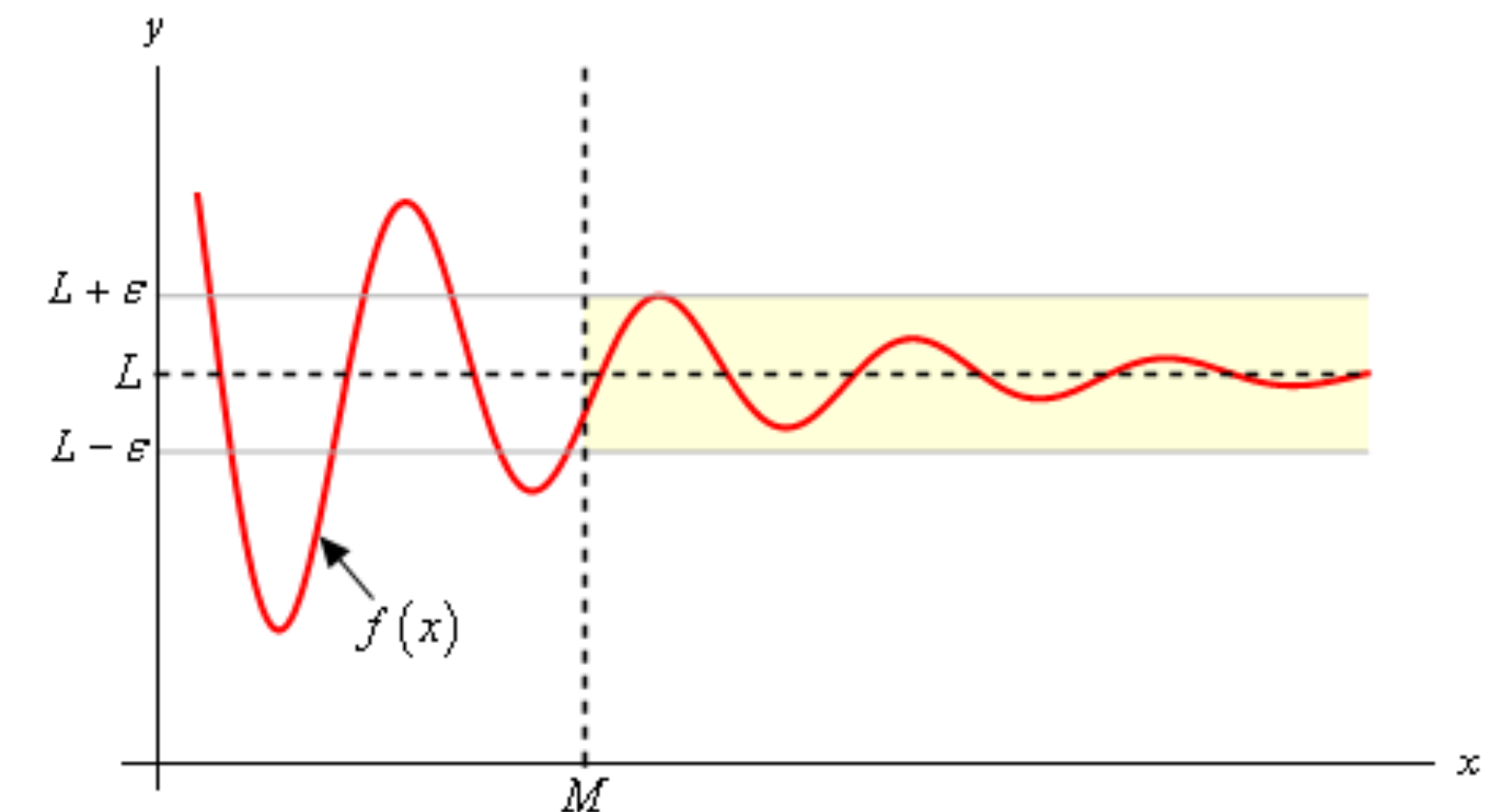
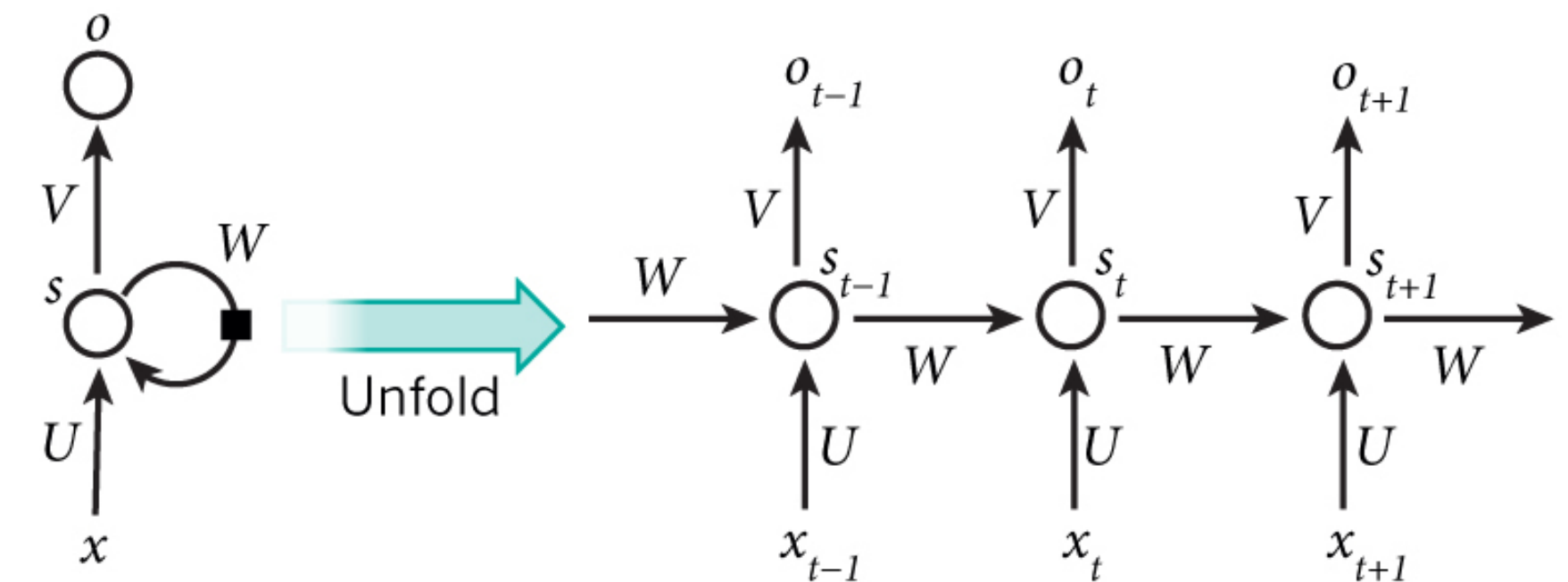




# MOTIVATION

- Optimization with inner loops
  - Meta learning, hyperparameter optimization
  - Recurrent models
- Optimization with limits
  - Discretized numerical methods: PDEs, ODEs, ...
  - Iterative methods: linear systems, inverses, eigenvalues,
  - Integration with Monte Carlo or quadrature
- In both cases..
  - cheap truncations/approximations cause **harmful bias**
  - accurate approximations are **computationally expensive**

$$\min_{\theta} \mathcal{L}(\theta) = \min_{\theta} \lim_{n \rightarrow H} \mathcal{L}_n(\theta)$$



# RANDOMIZED TELESCOPES: UNBIASED ESTIMATION OF LIMITS

Consider:  $Y_H := \lim_{n \rightarrow H} Y_n$

Then:  $Y_H = \sum_{n=1}^H \Delta_n$  where  $\Delta_n = \begin{cases} Y_n - Y_{n-1} & n > 1 \\ Y_1 & n = 1 \end{cases}$

Consider an estimator:  $\hat{Y}_H = \sum_{n=1}^N \Delta_n W(n, N) \quad N \in \{1, \dots, H\} \sim q$

This is unbiased iff:  $\sum_{N=n}^H W(n, N) q(N) = 1 \quad \forall n$



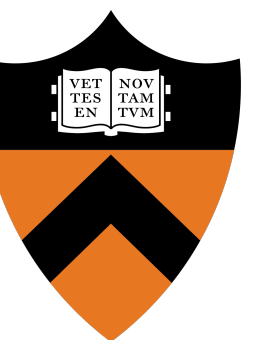
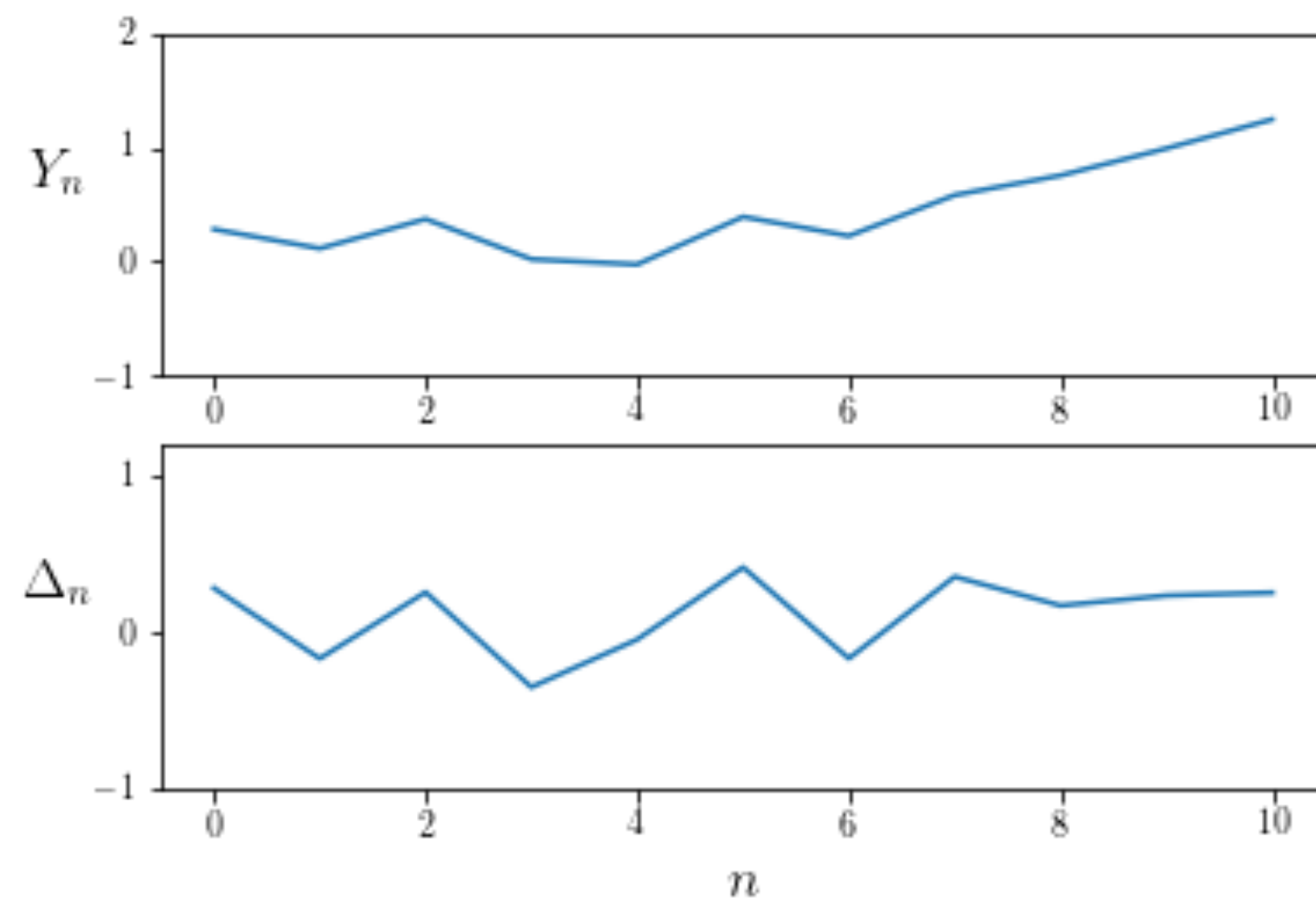
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Ground truth



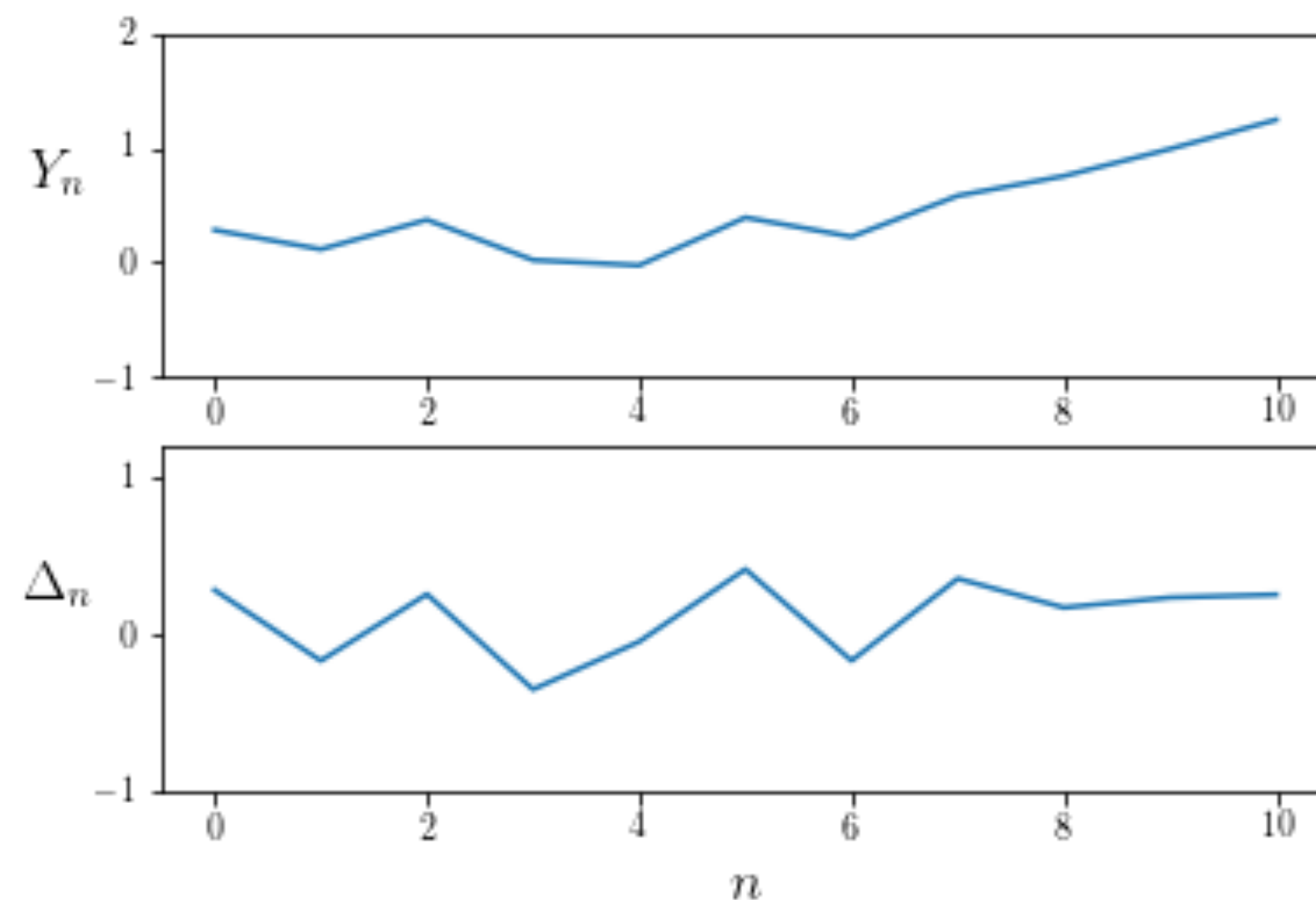
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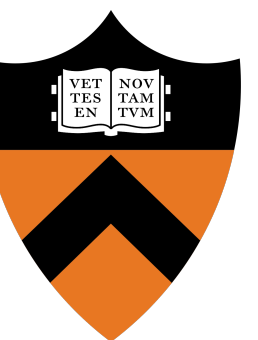


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$$W(n, N) = \frac{1}{q(N)} \mathbb{1}\{n = N\}$$

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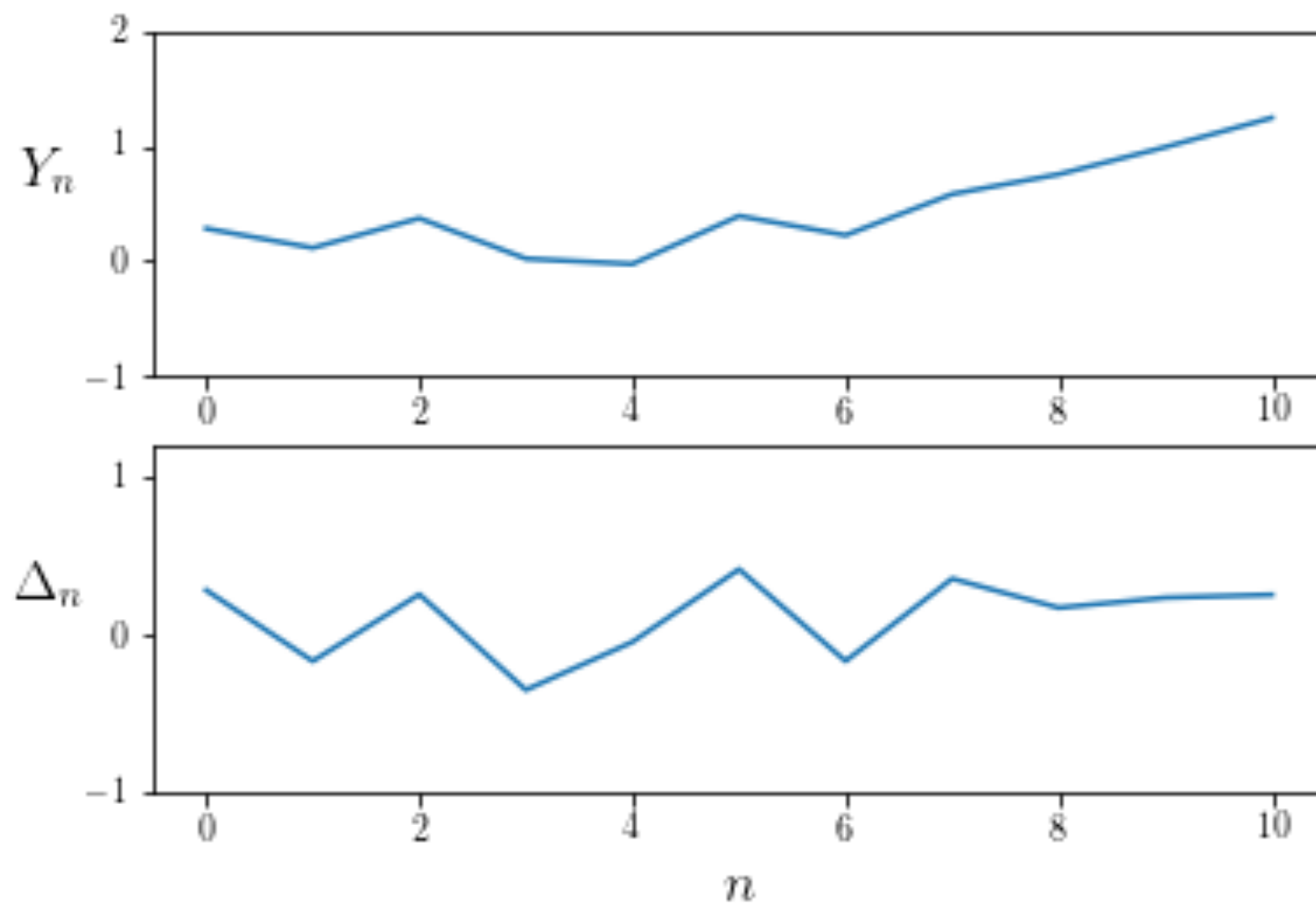
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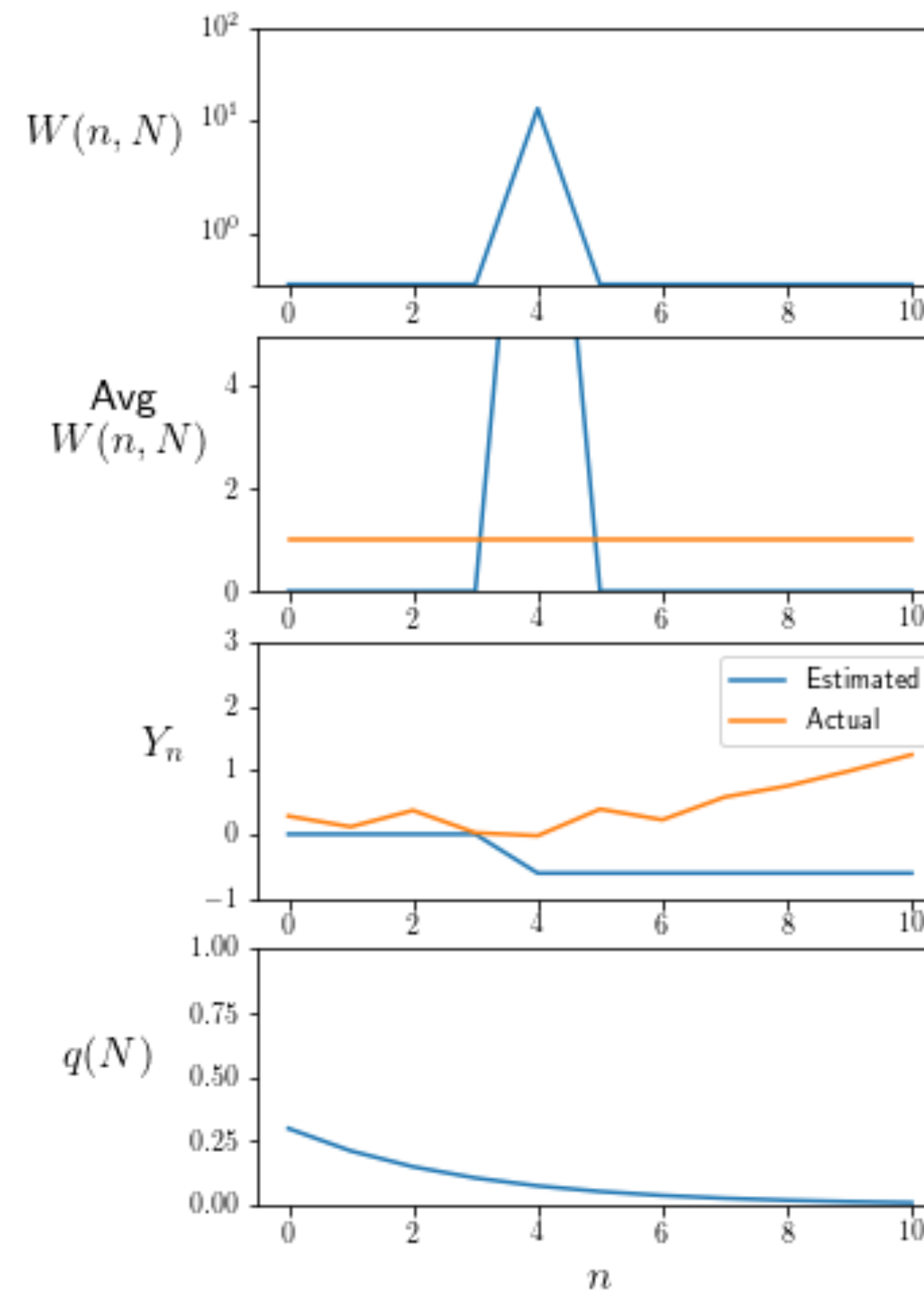
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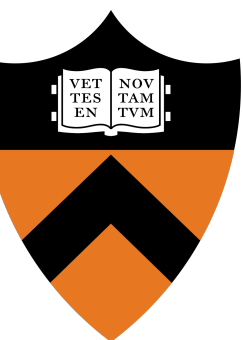
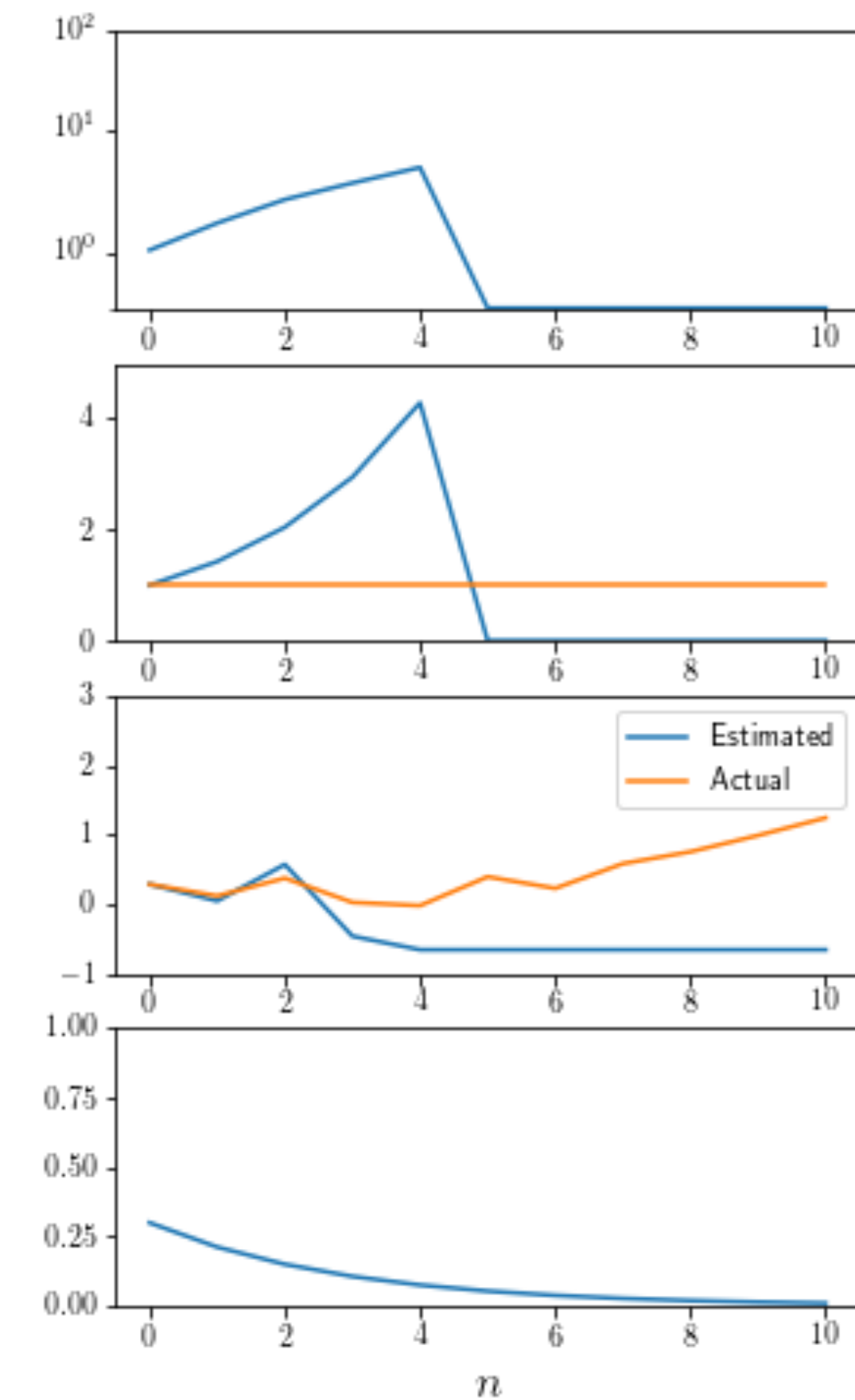
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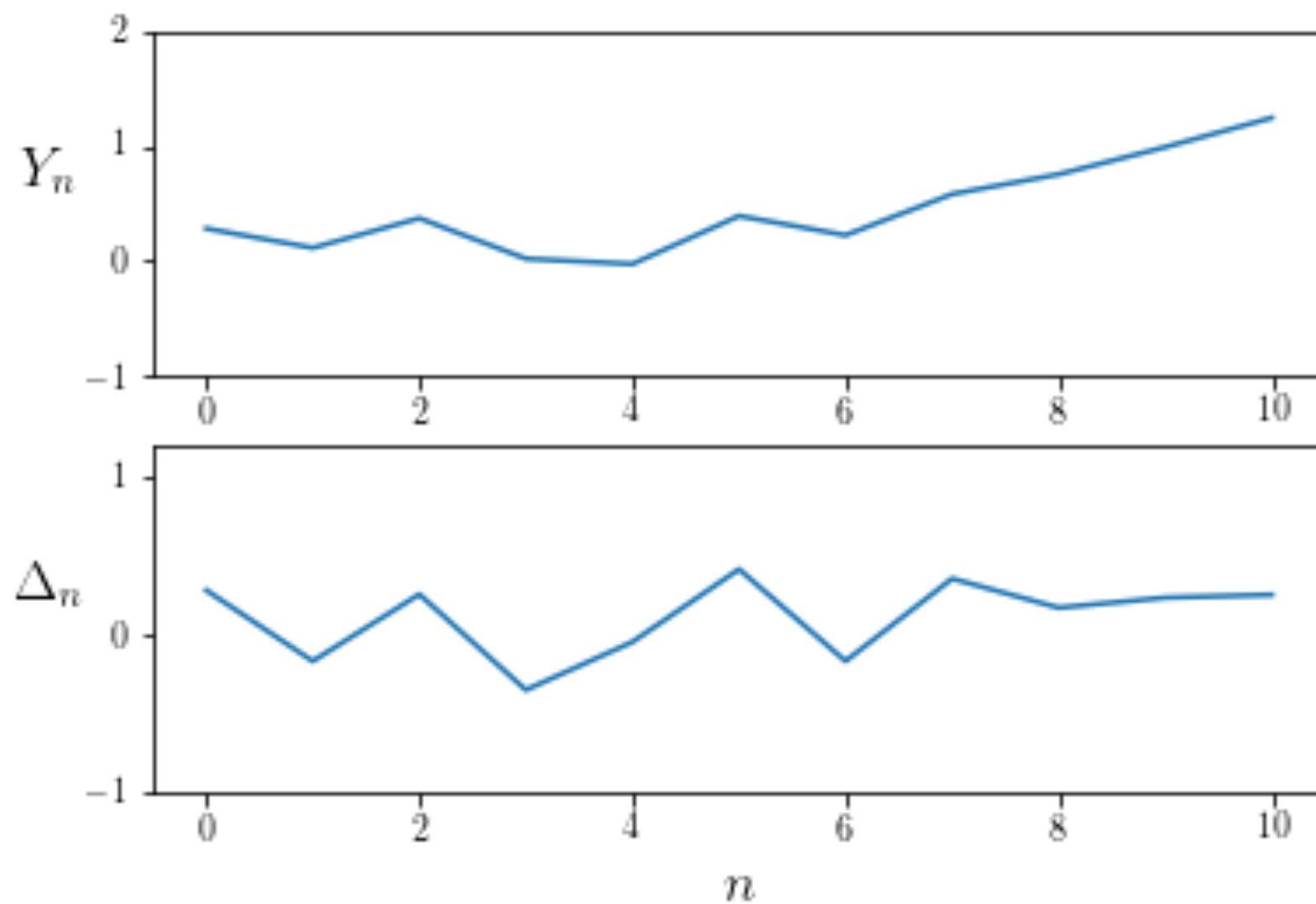
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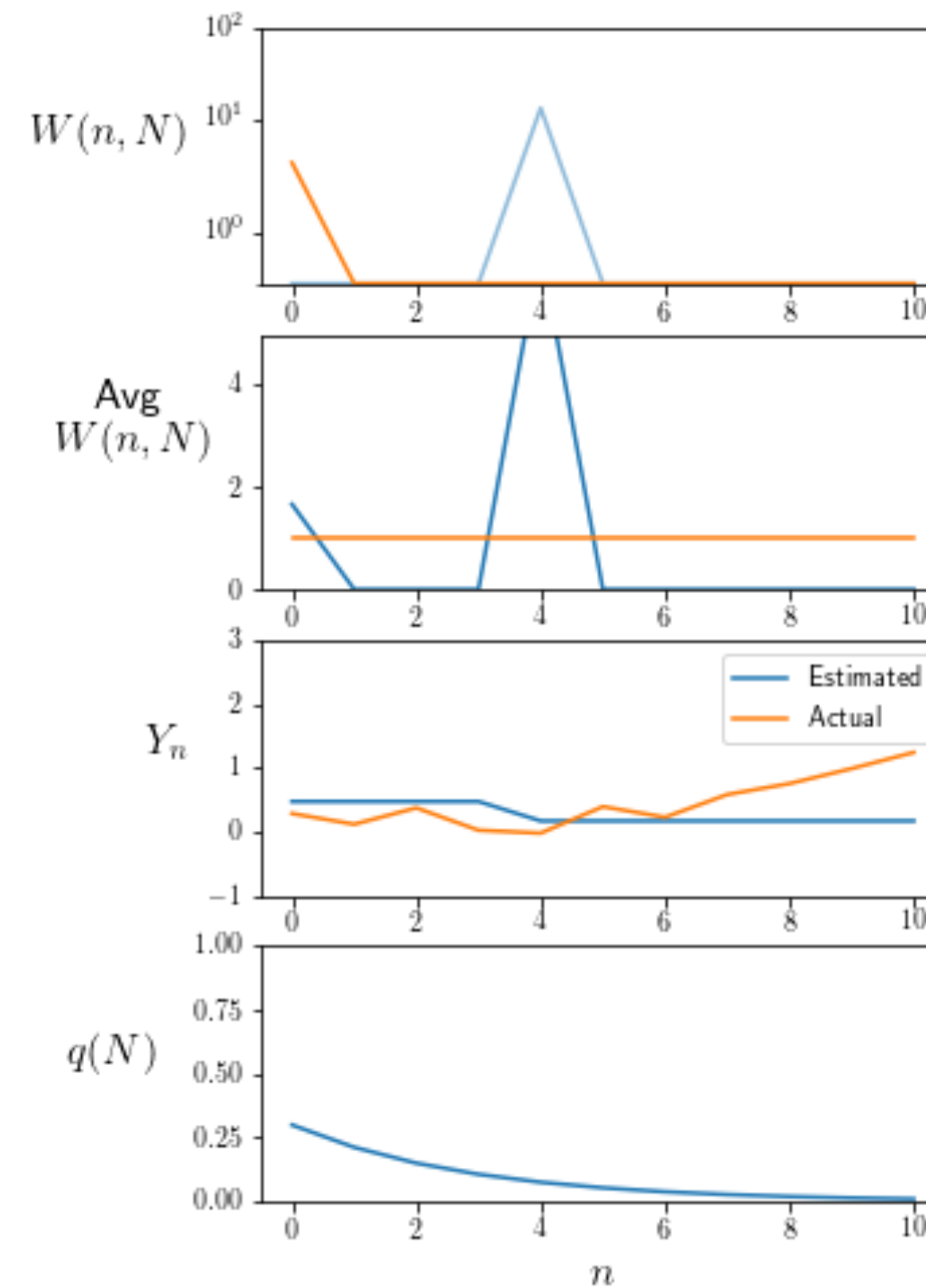
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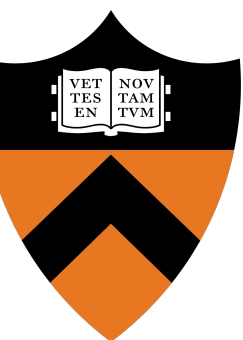
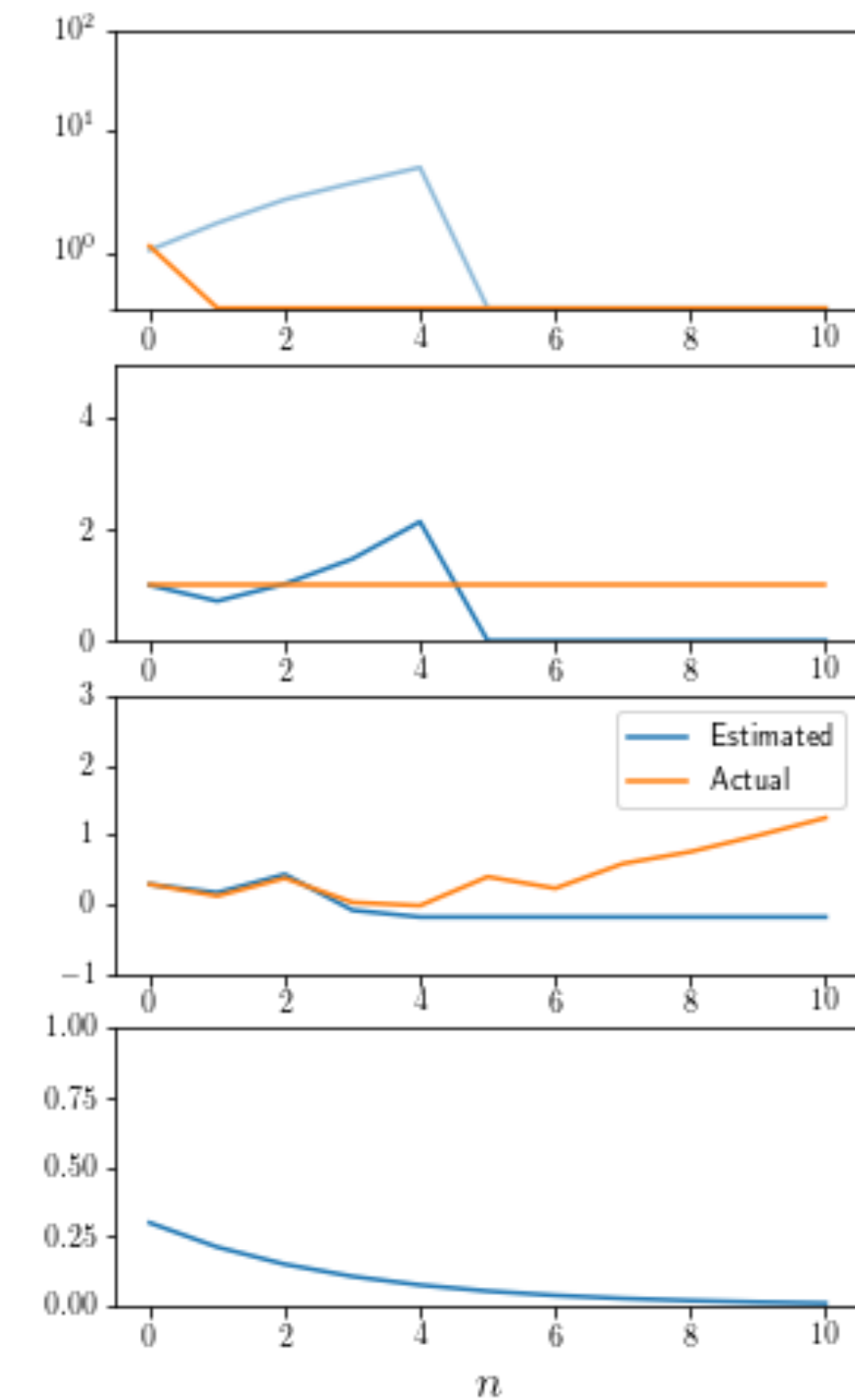
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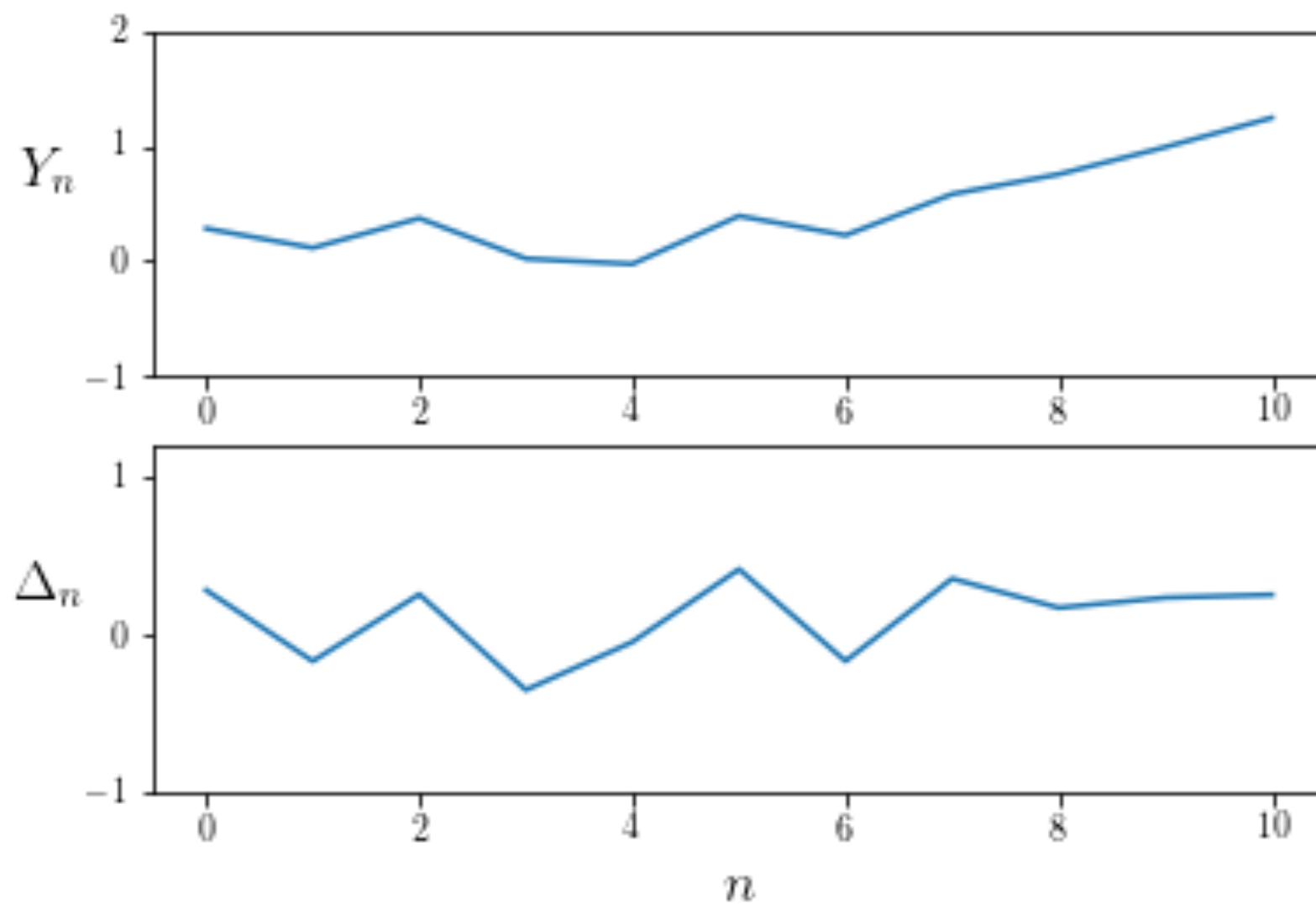
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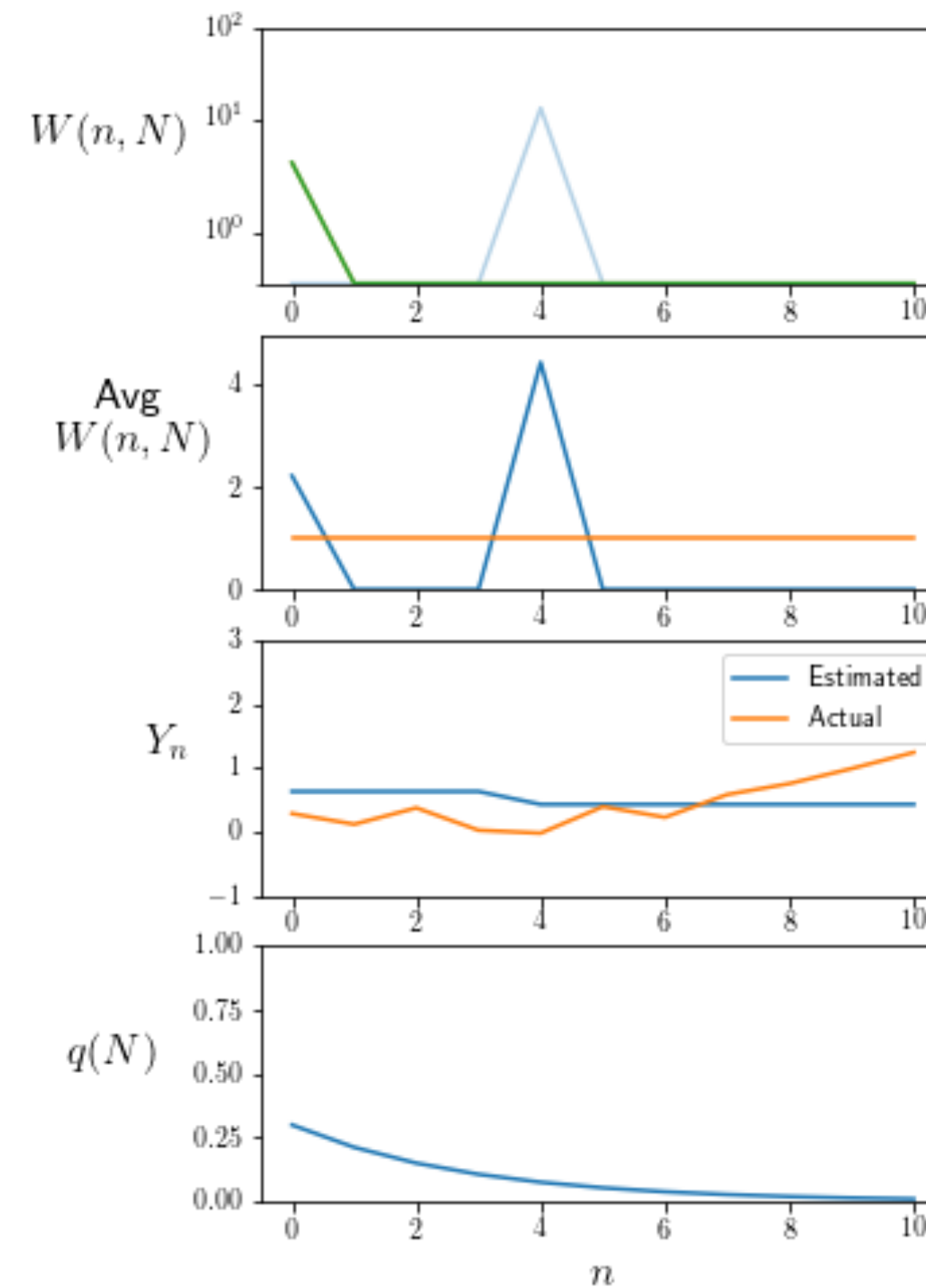
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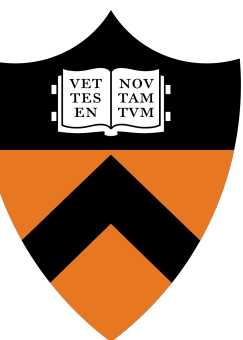
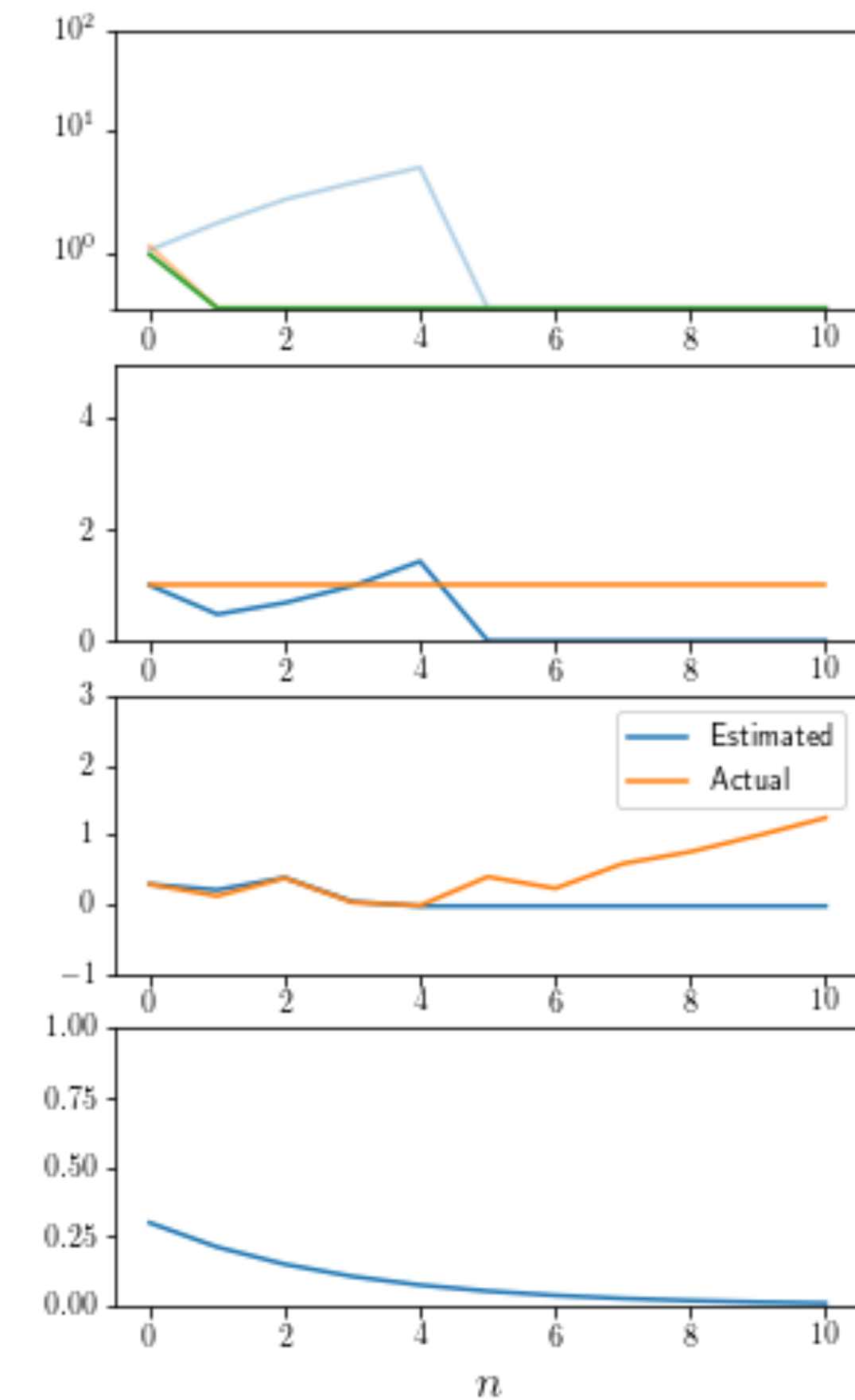
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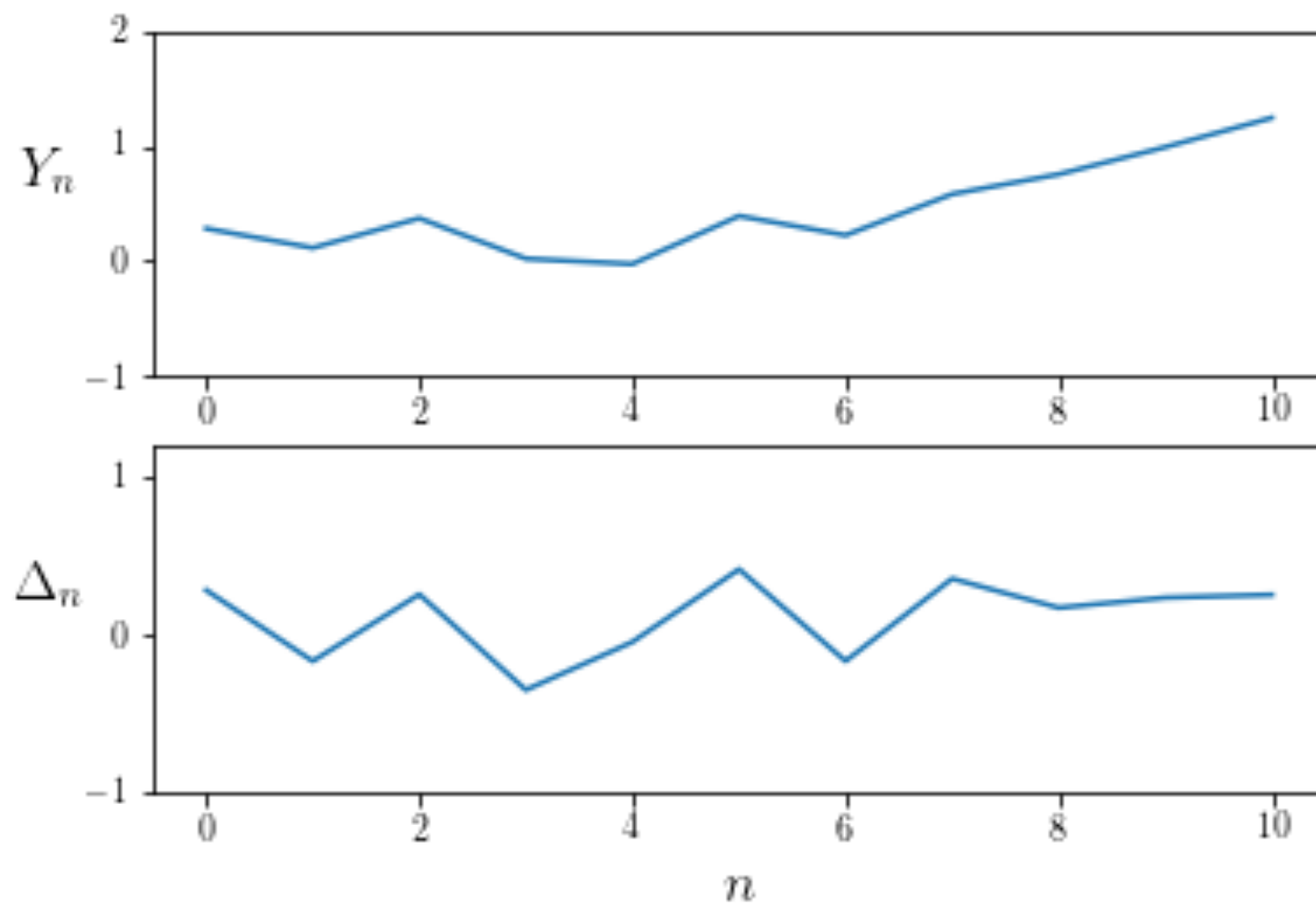
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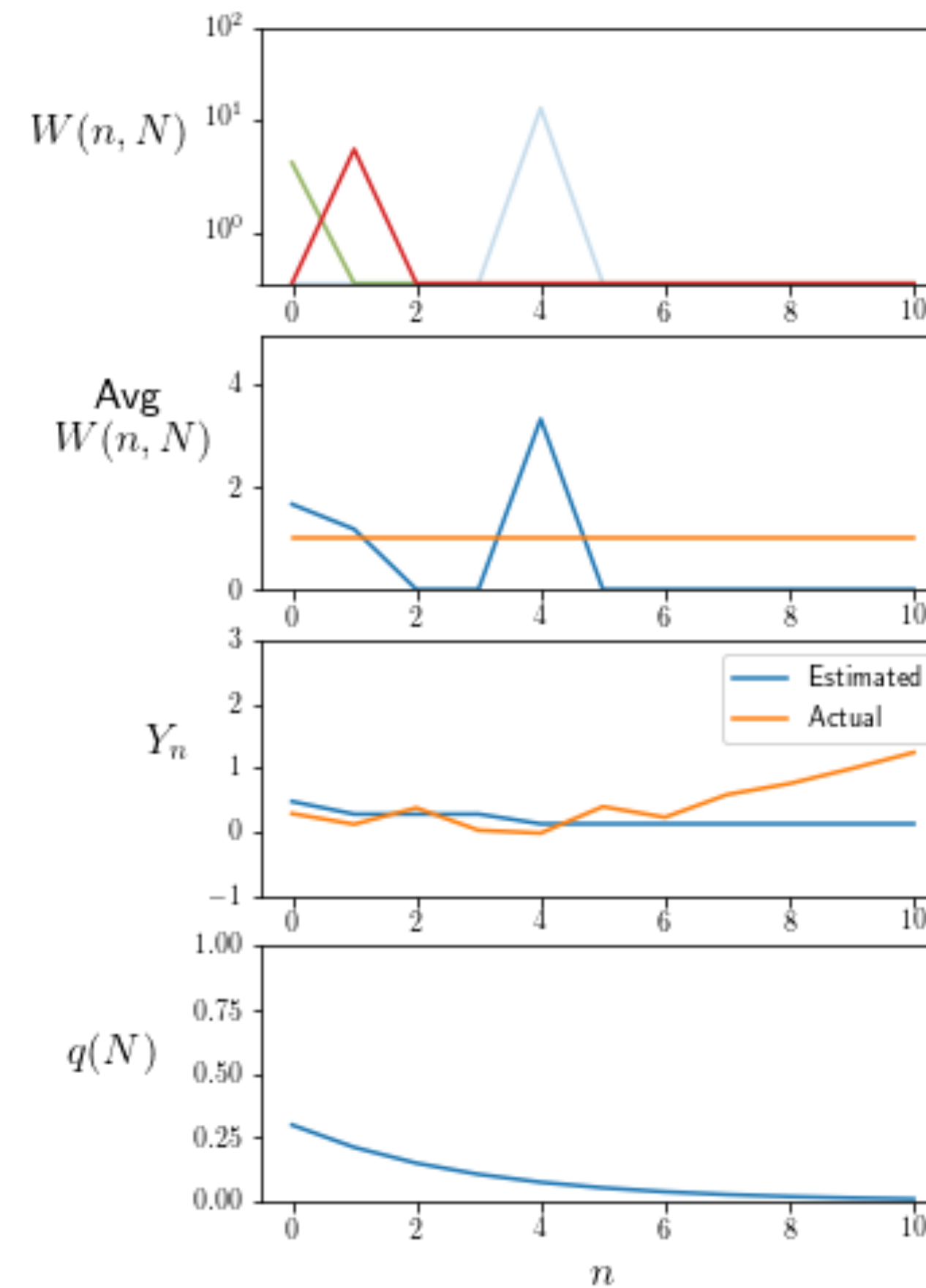
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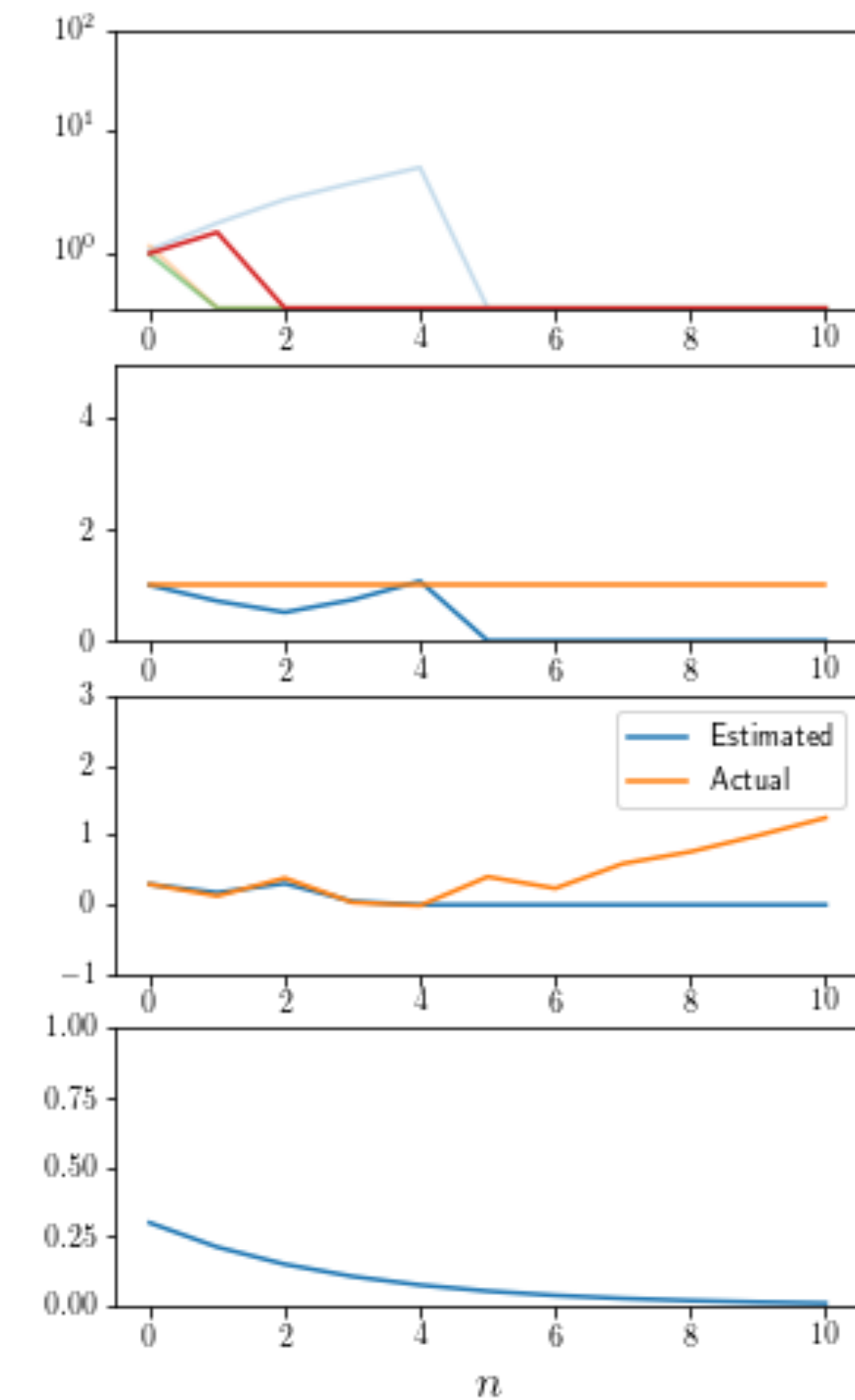
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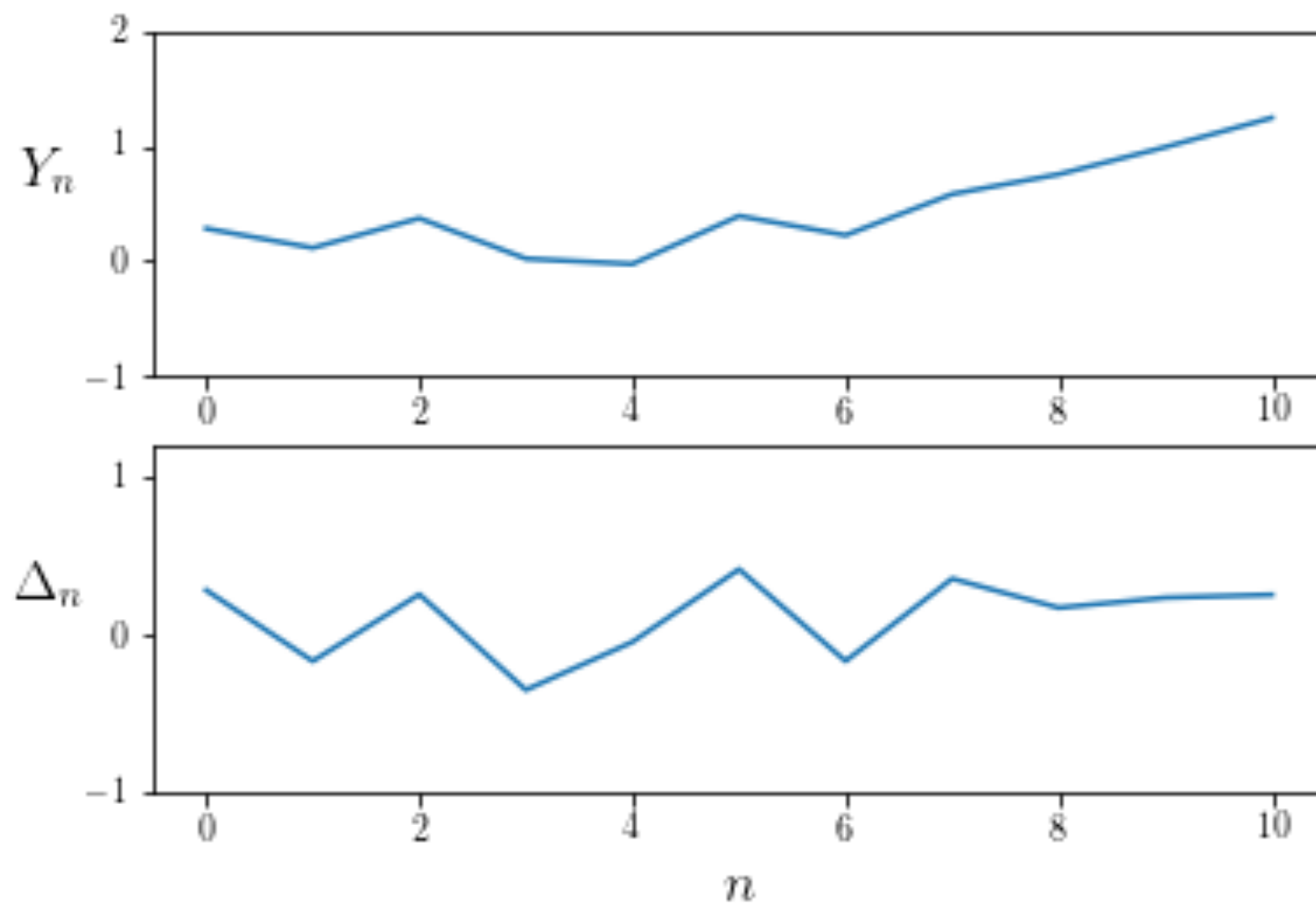
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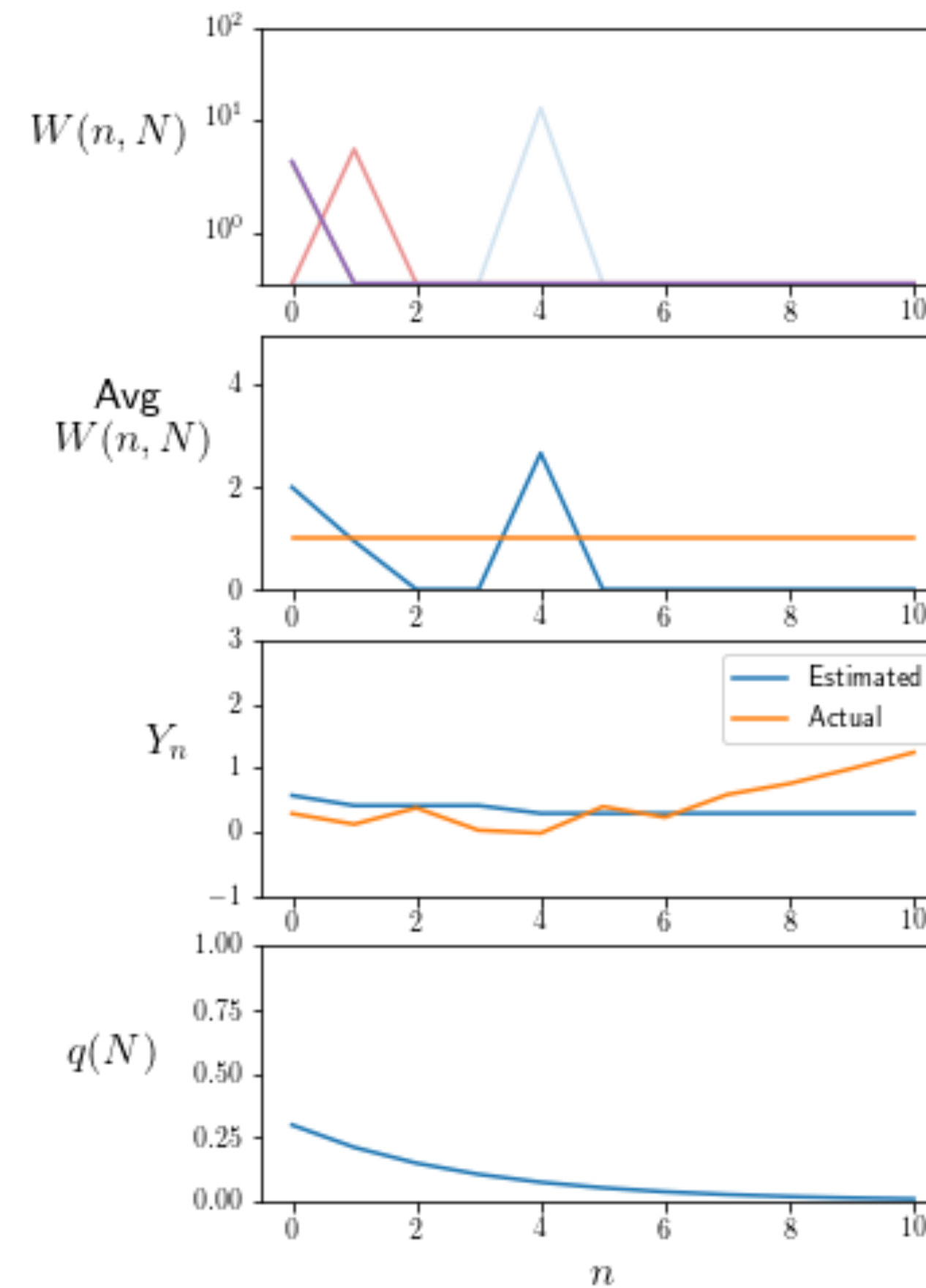
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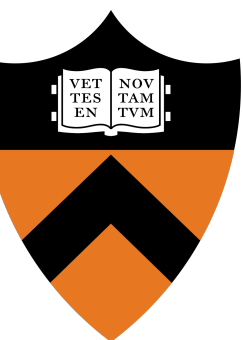
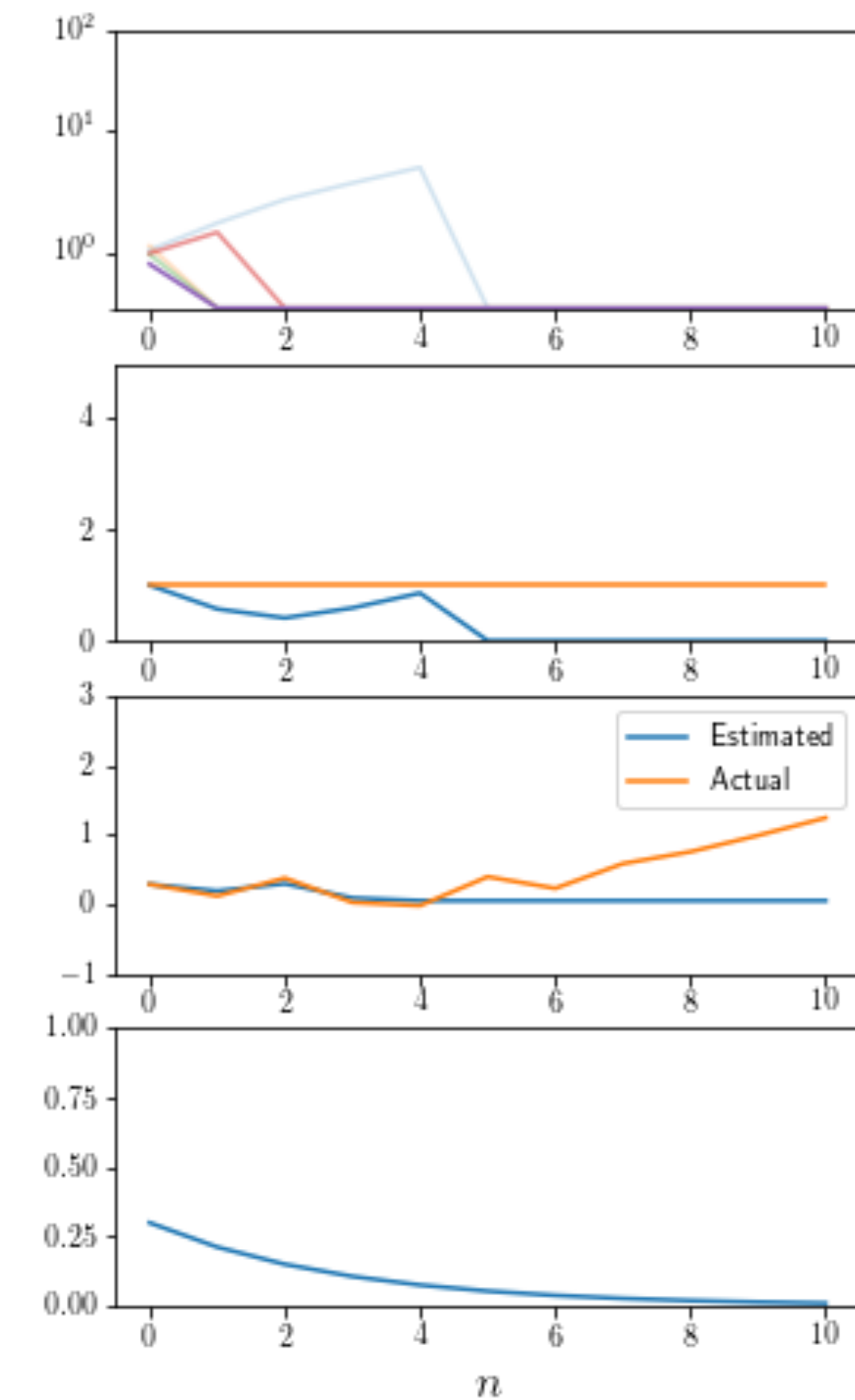
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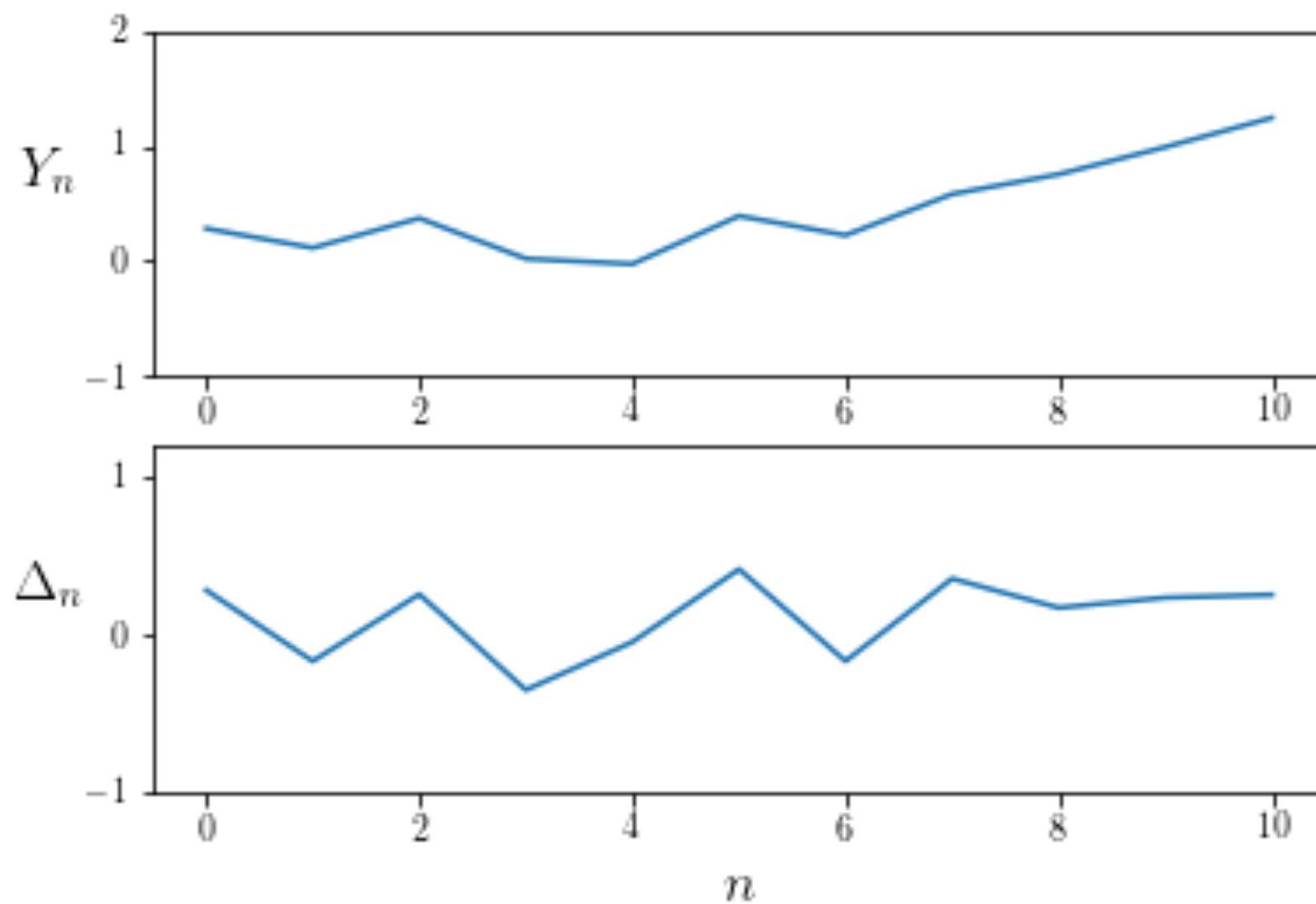
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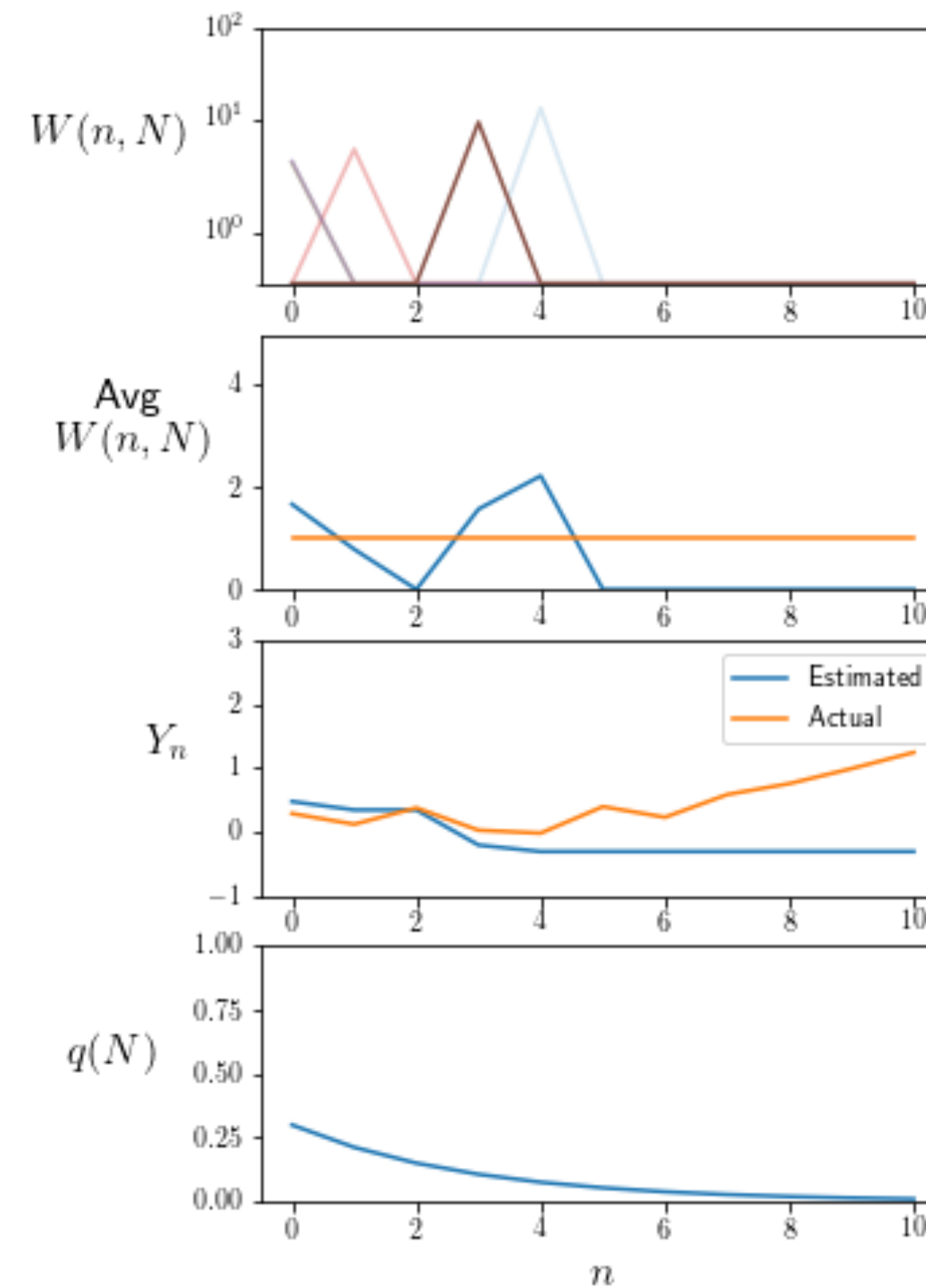
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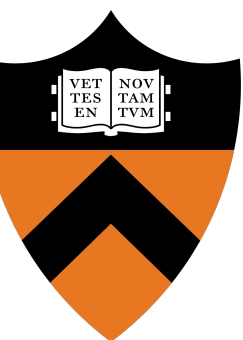
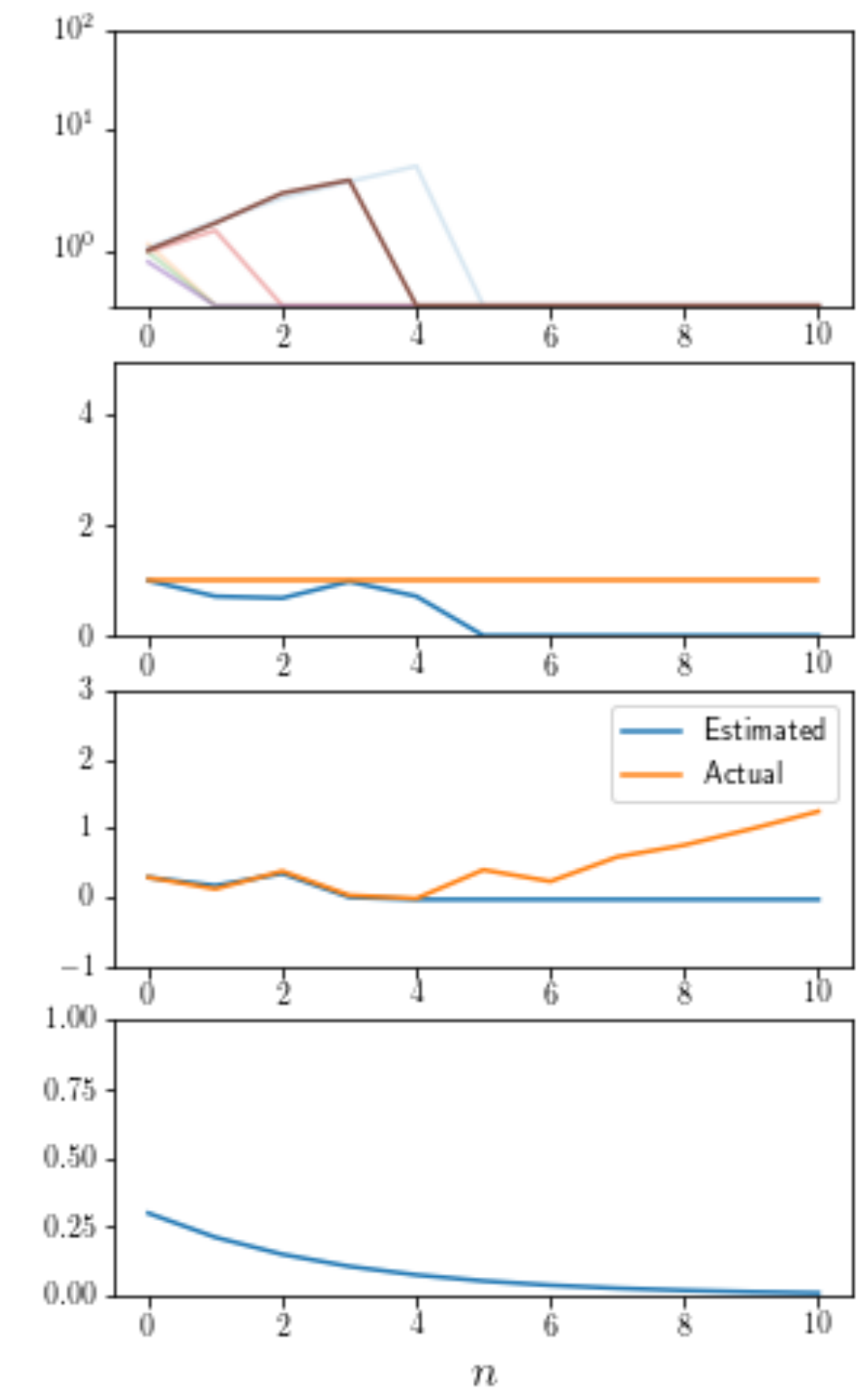
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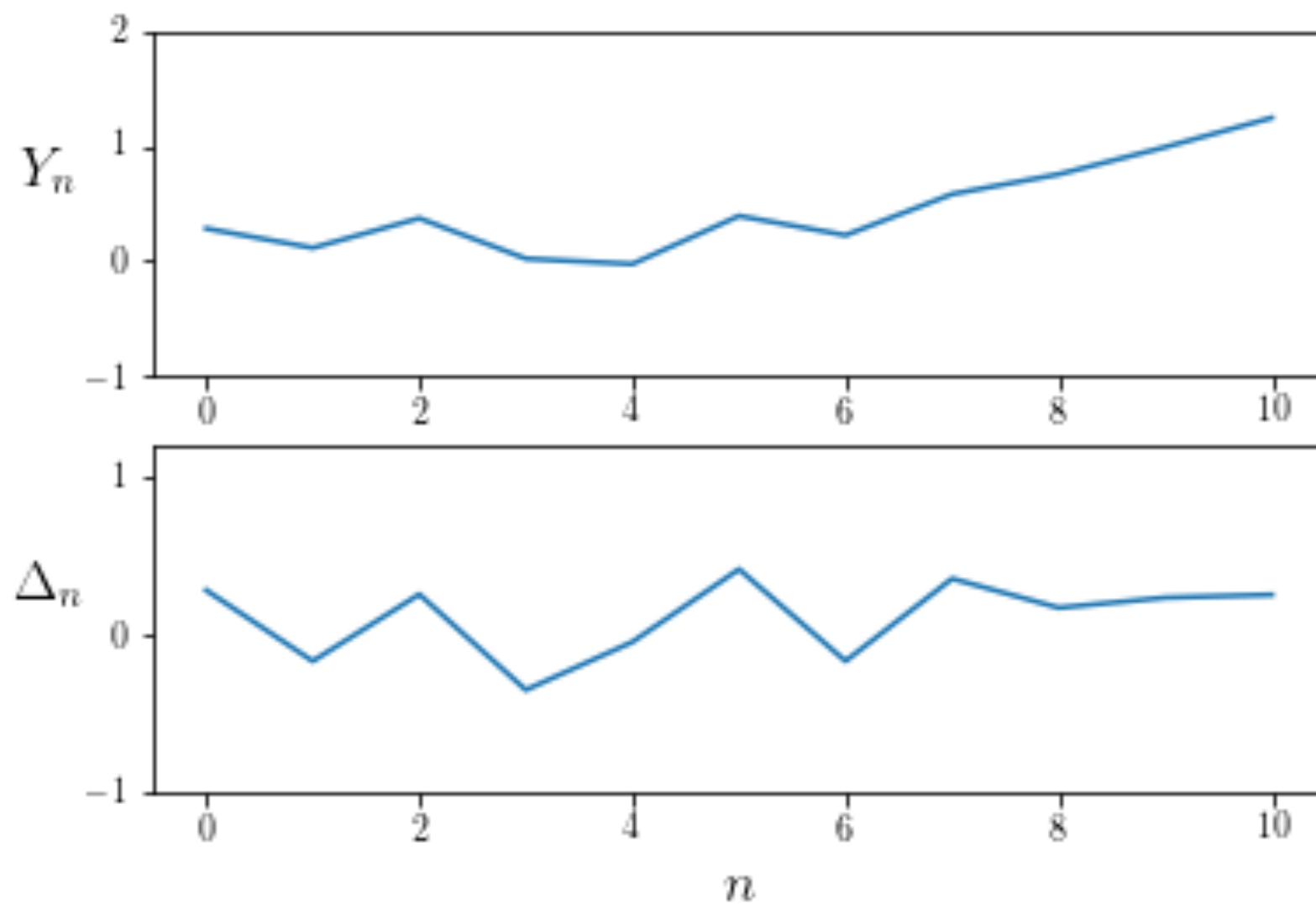
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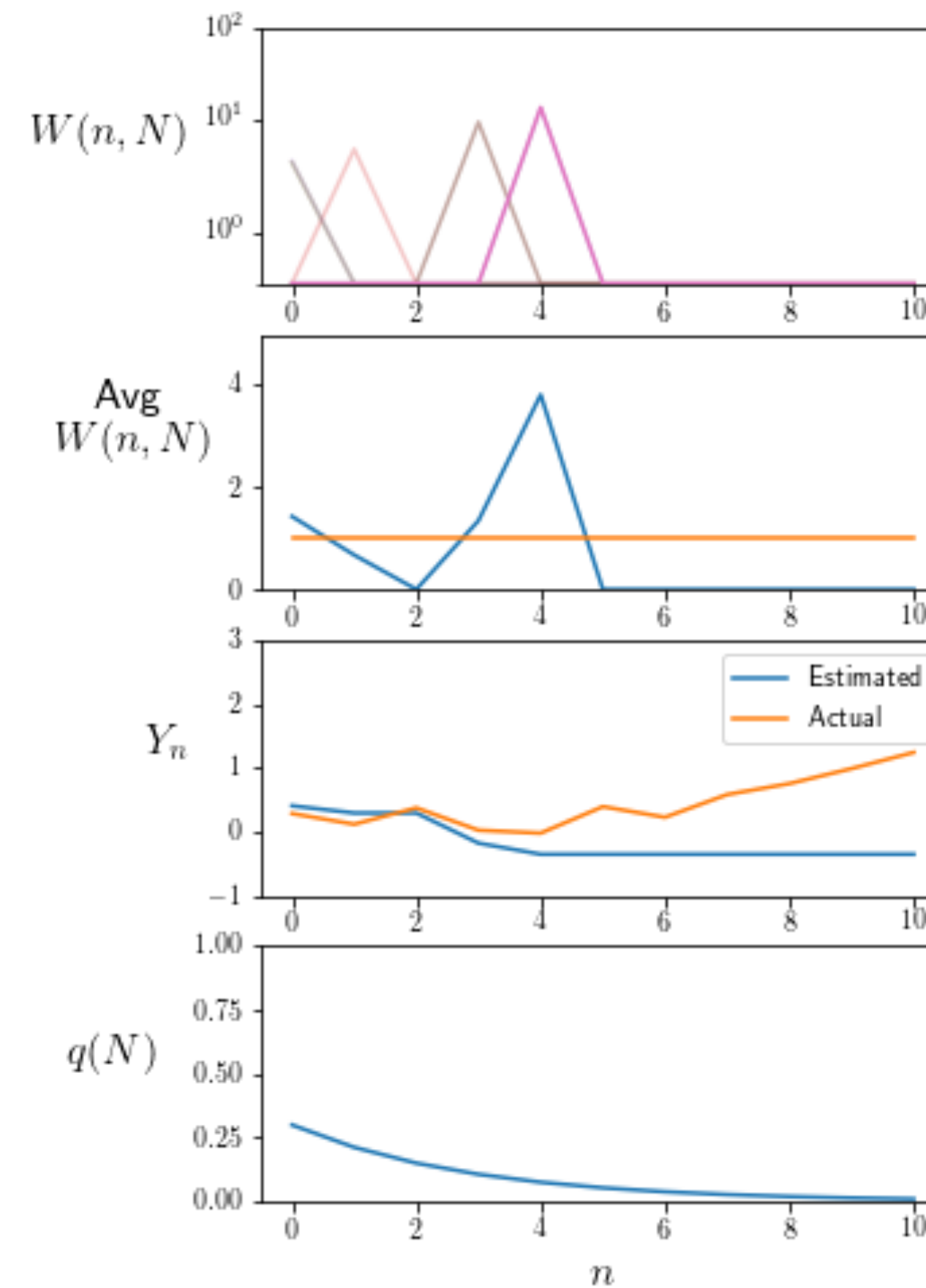
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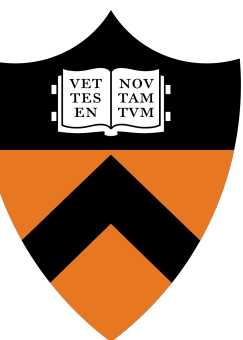
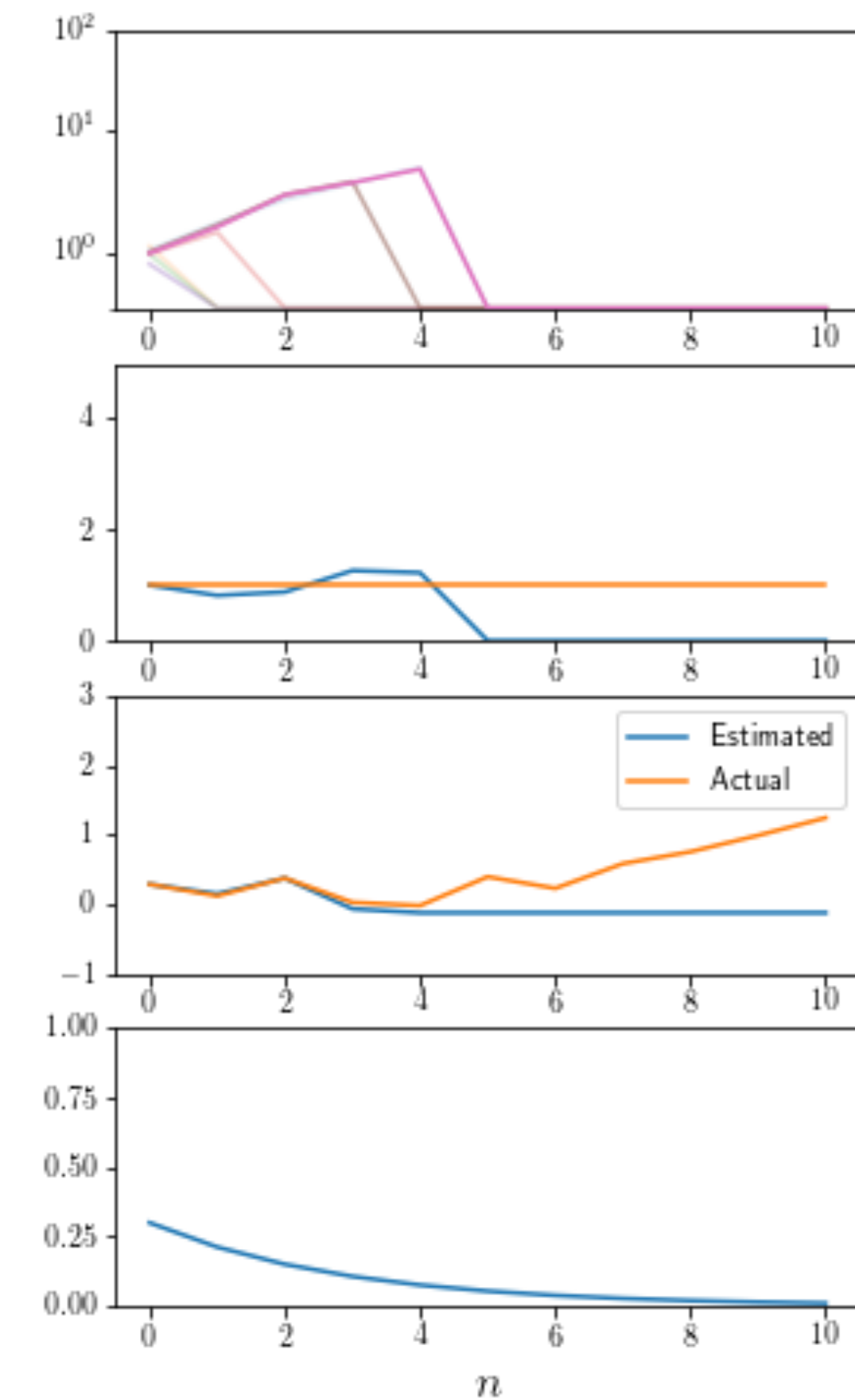
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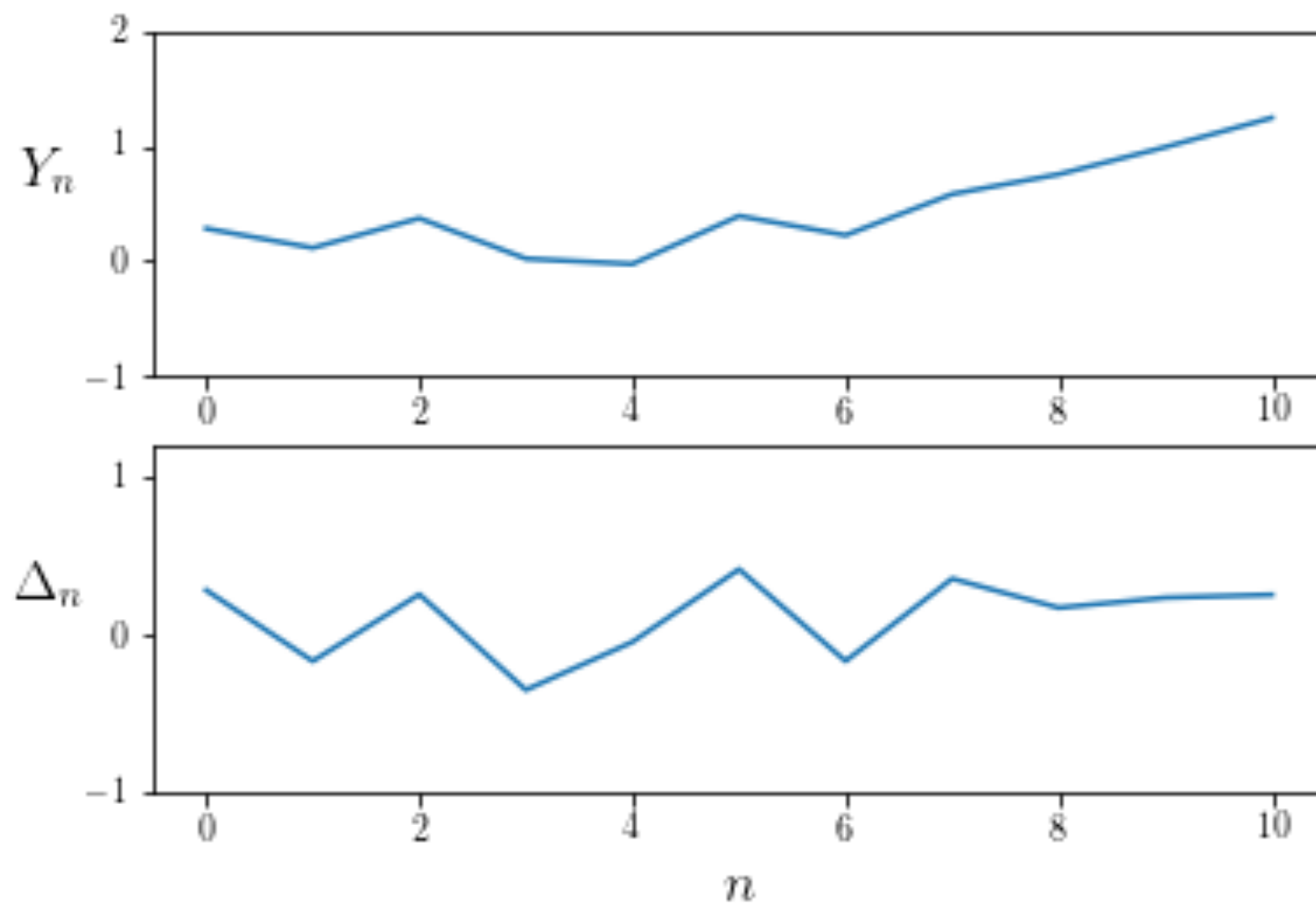
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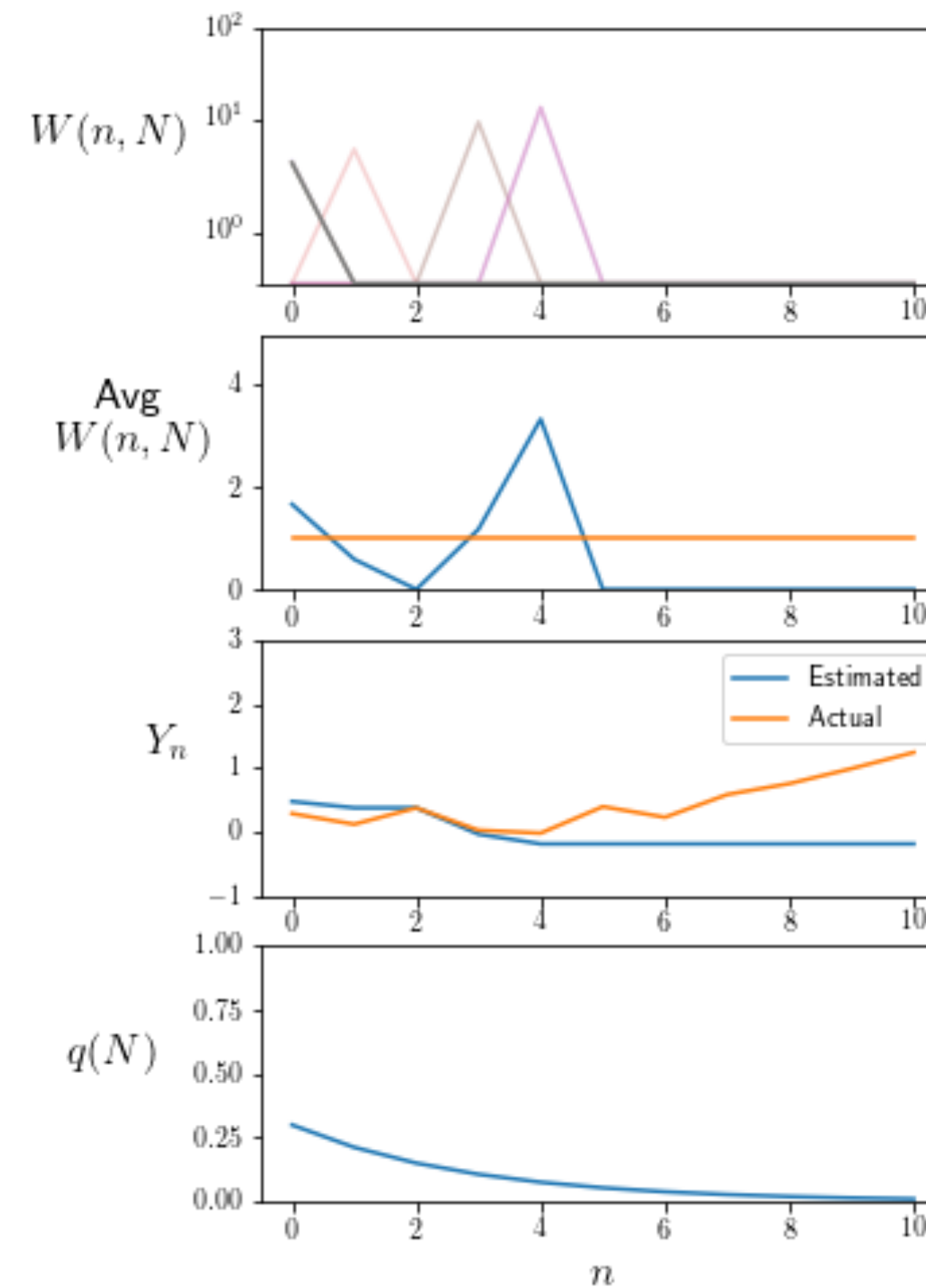
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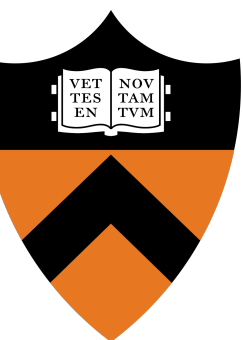
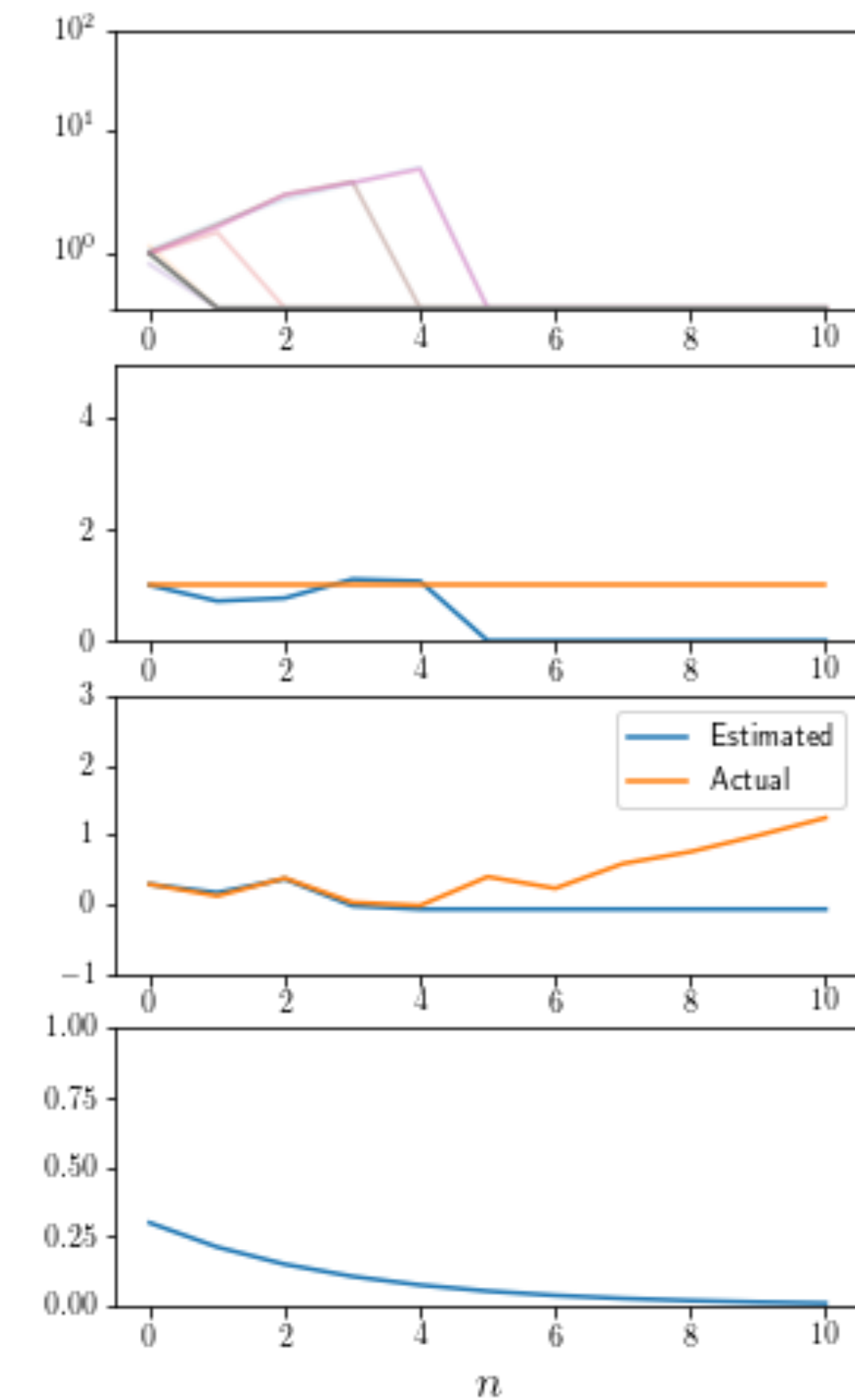
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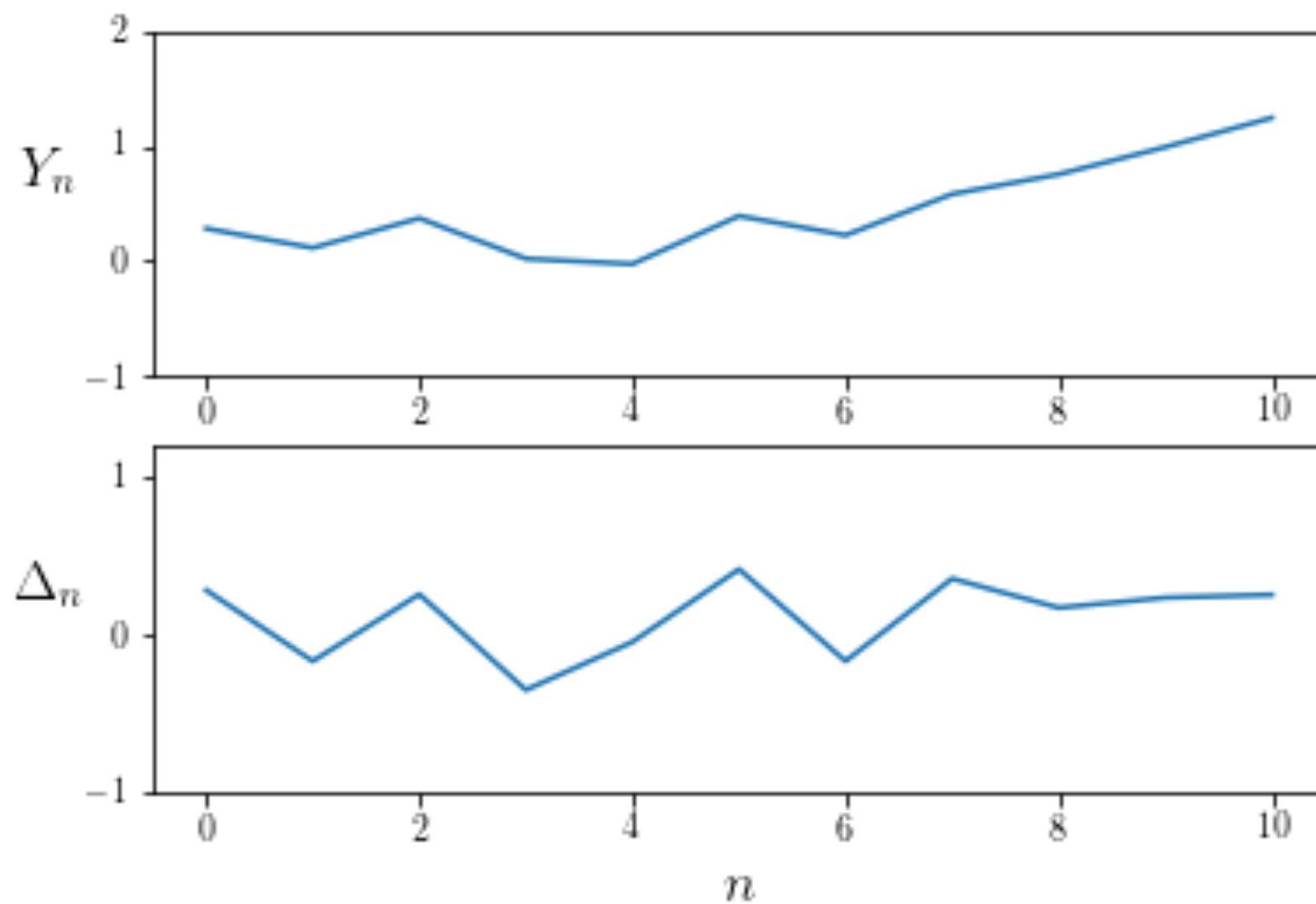
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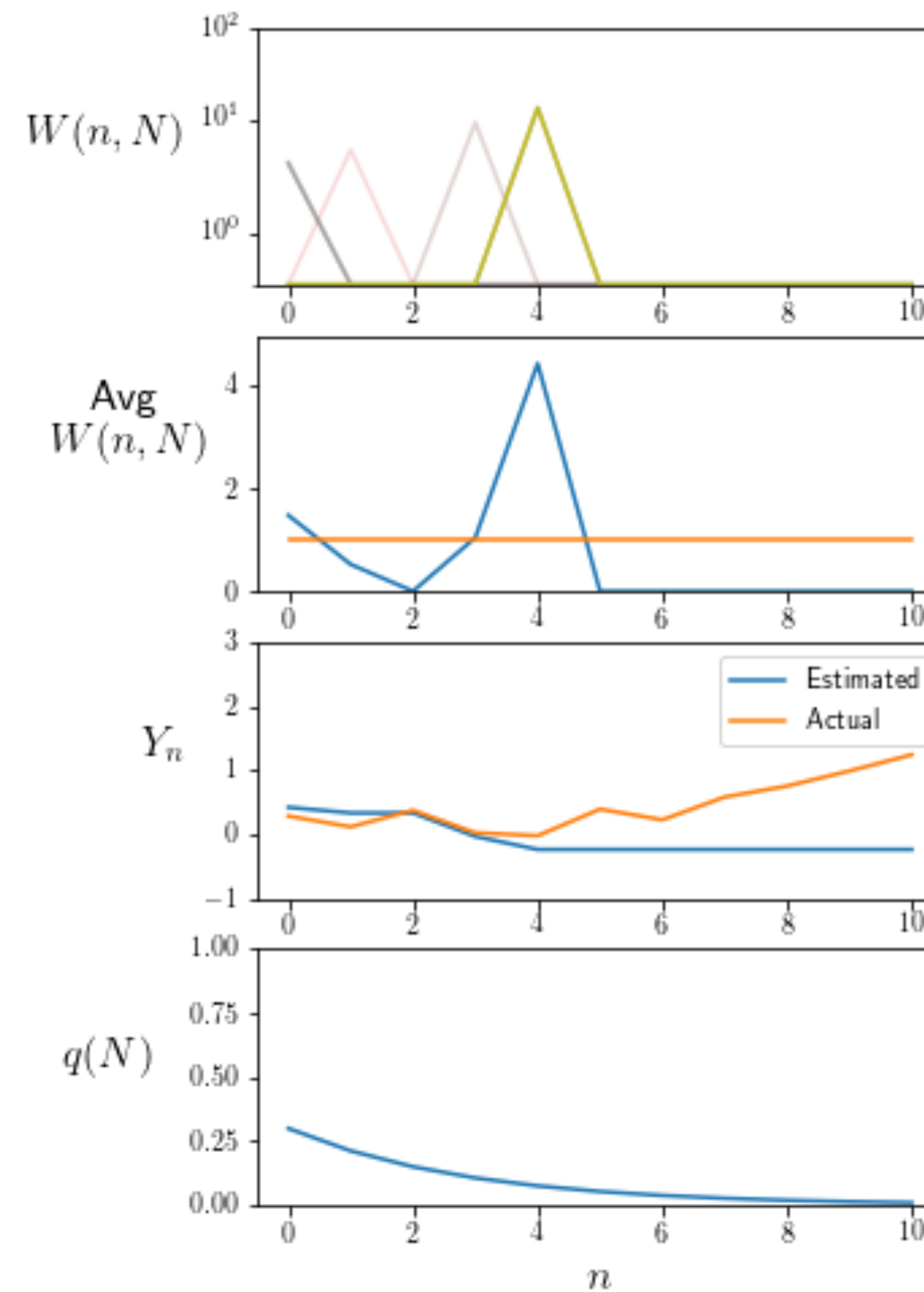
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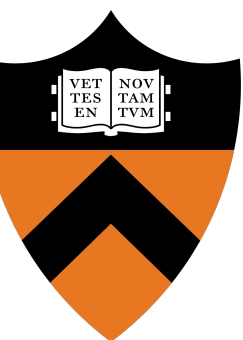
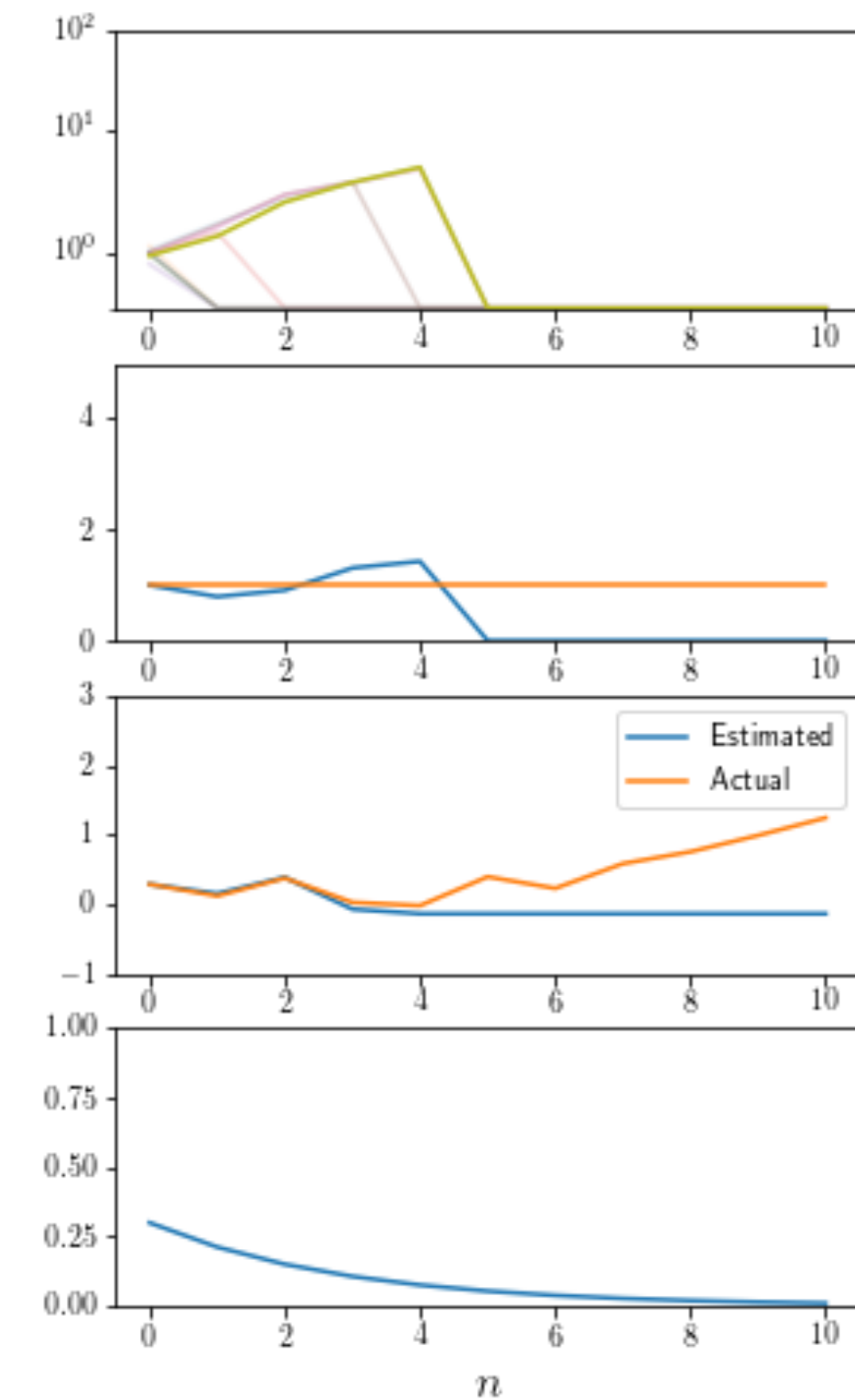
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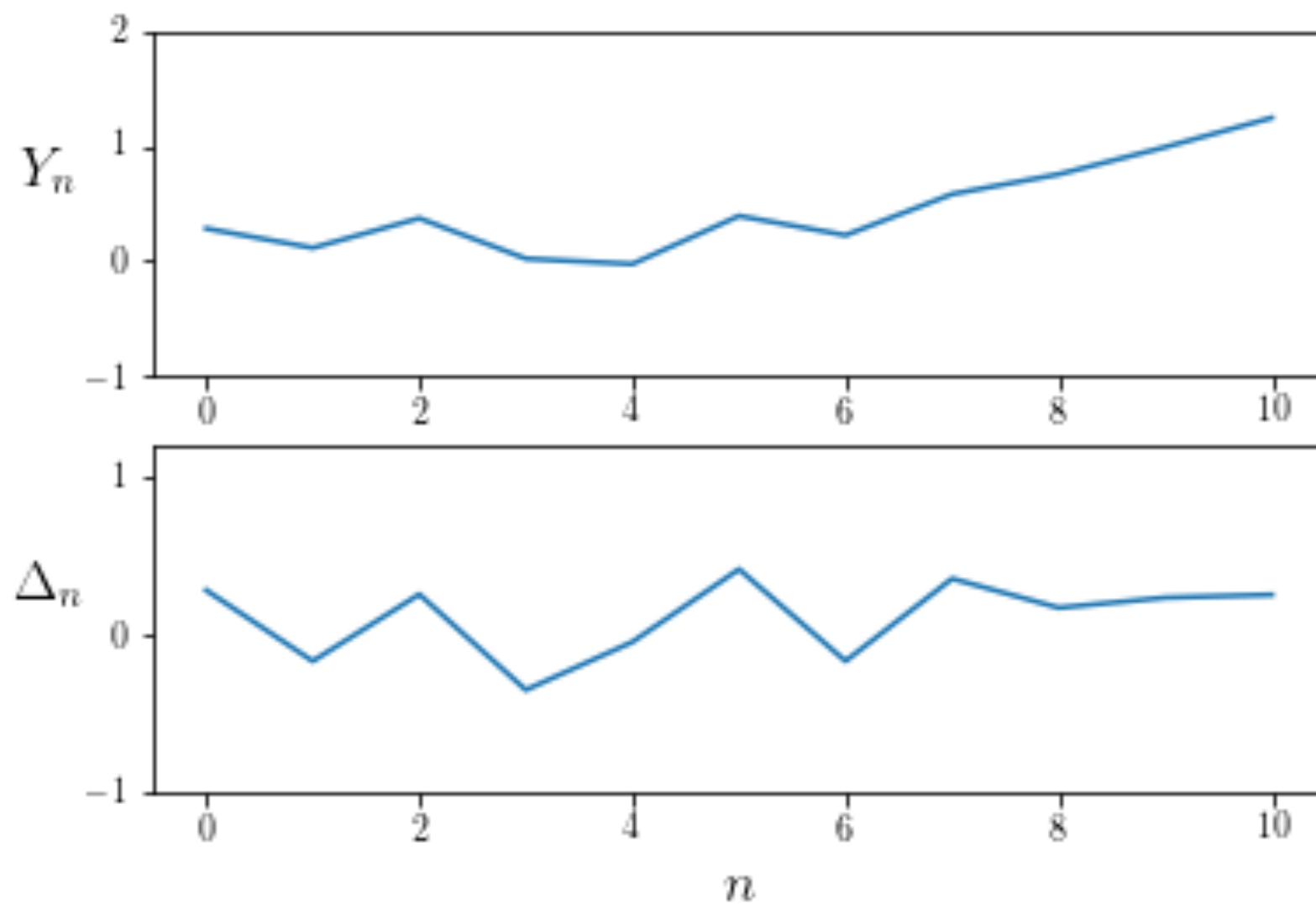
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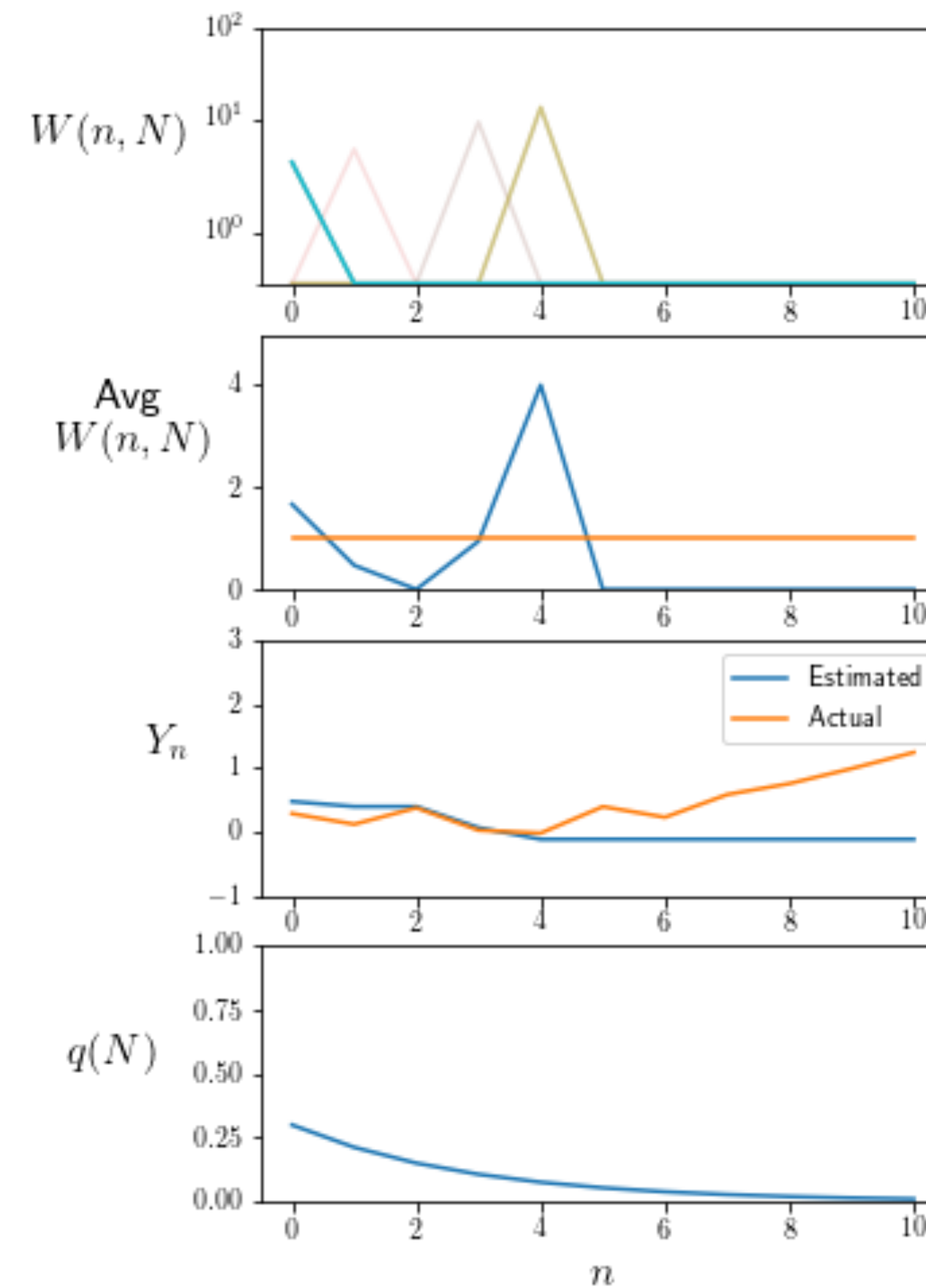
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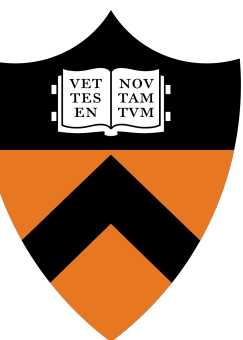
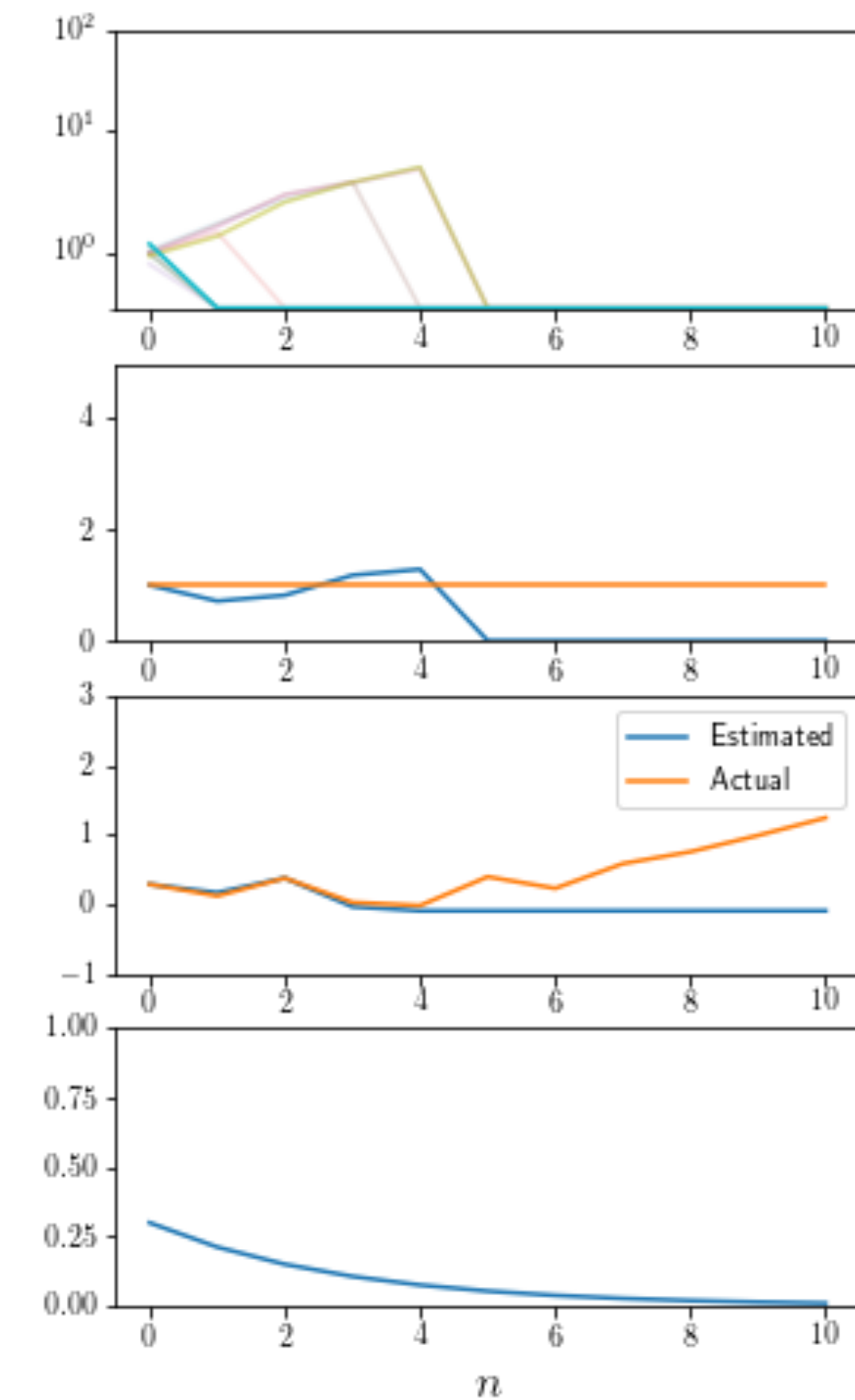
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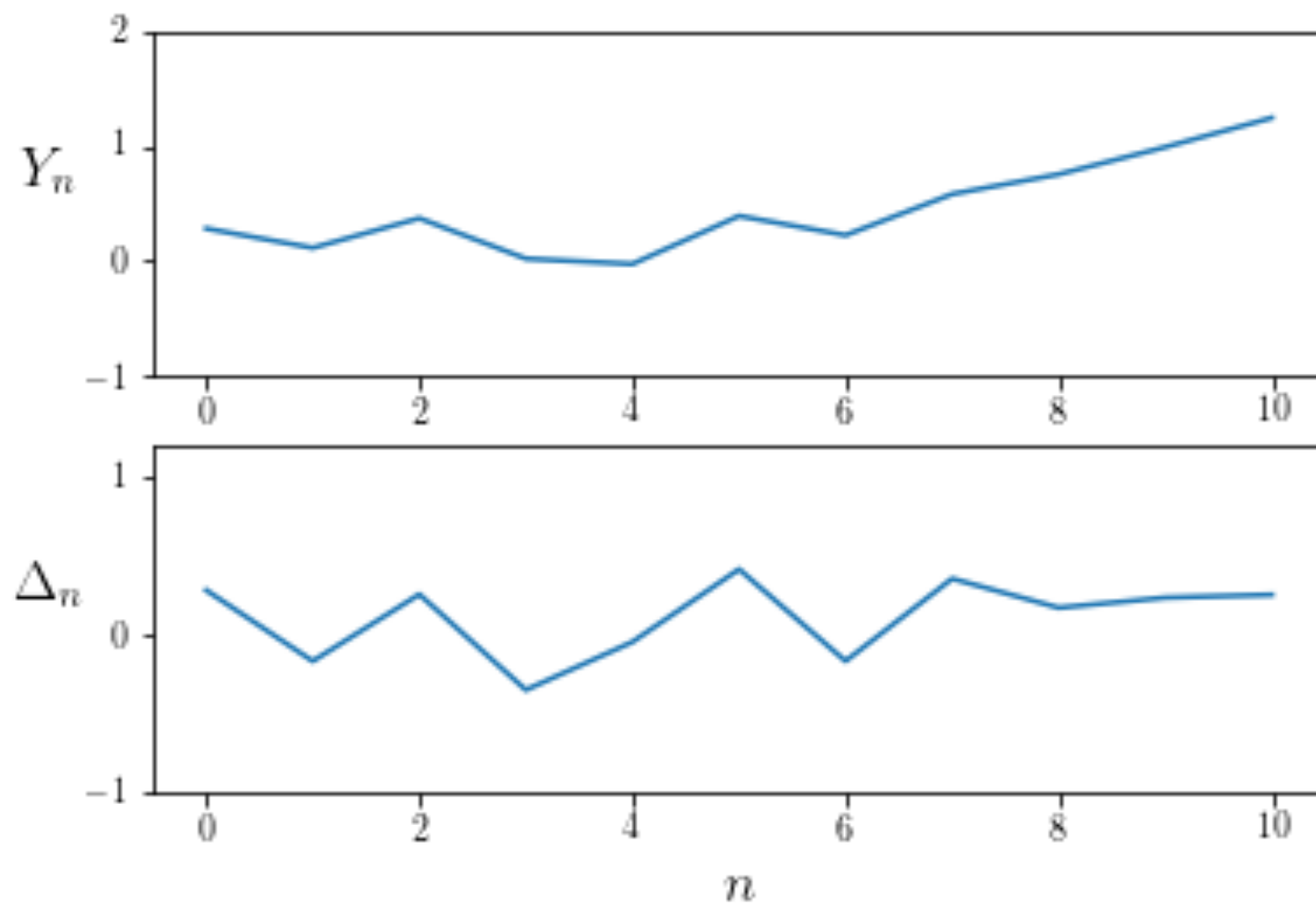
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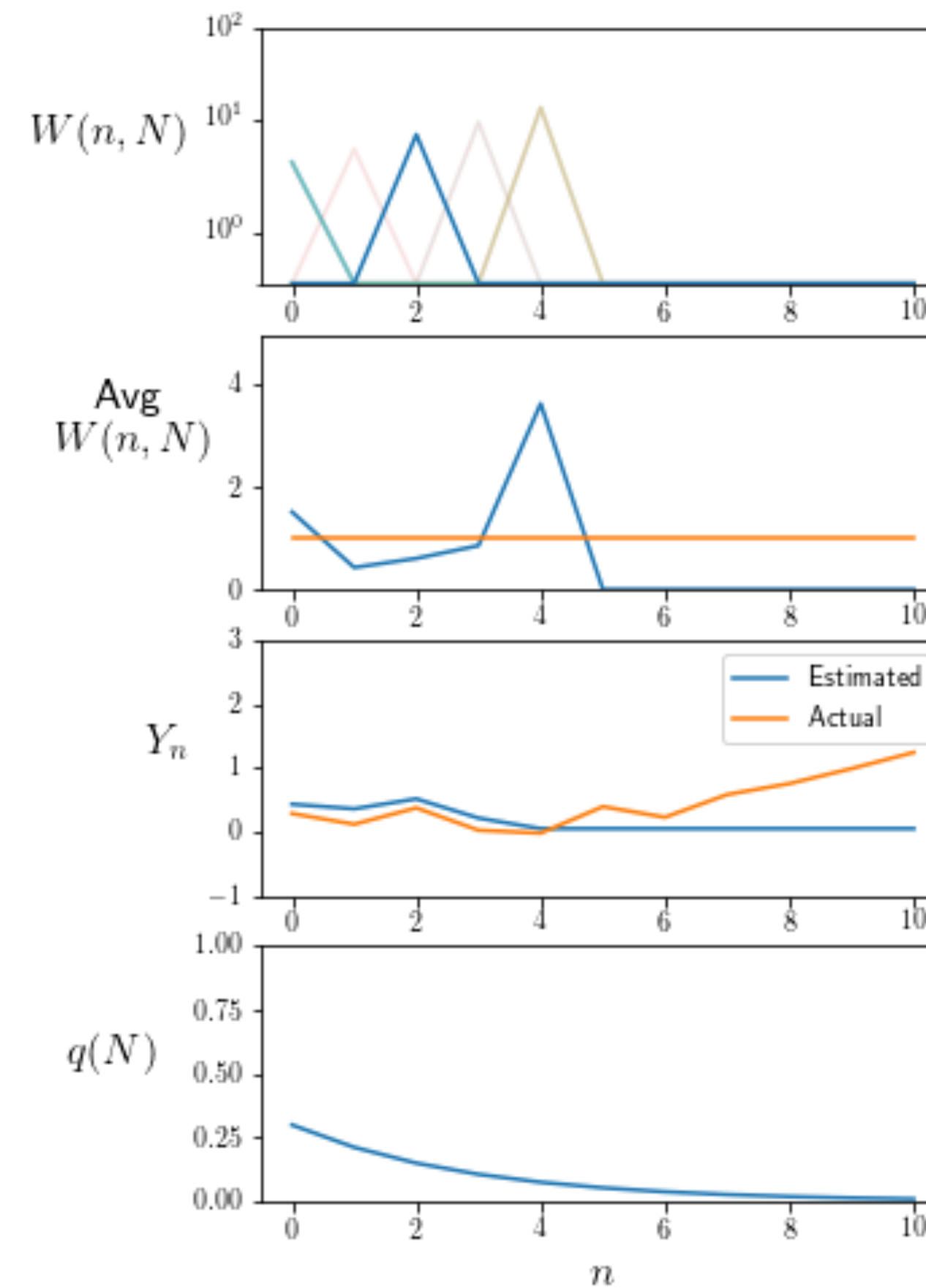
$$\Delta_n = \begin{cases} Y_n - Y_{n-1} & n > 1 \\ Y_1 & n = 1 \end{cases}$$

Ground truth



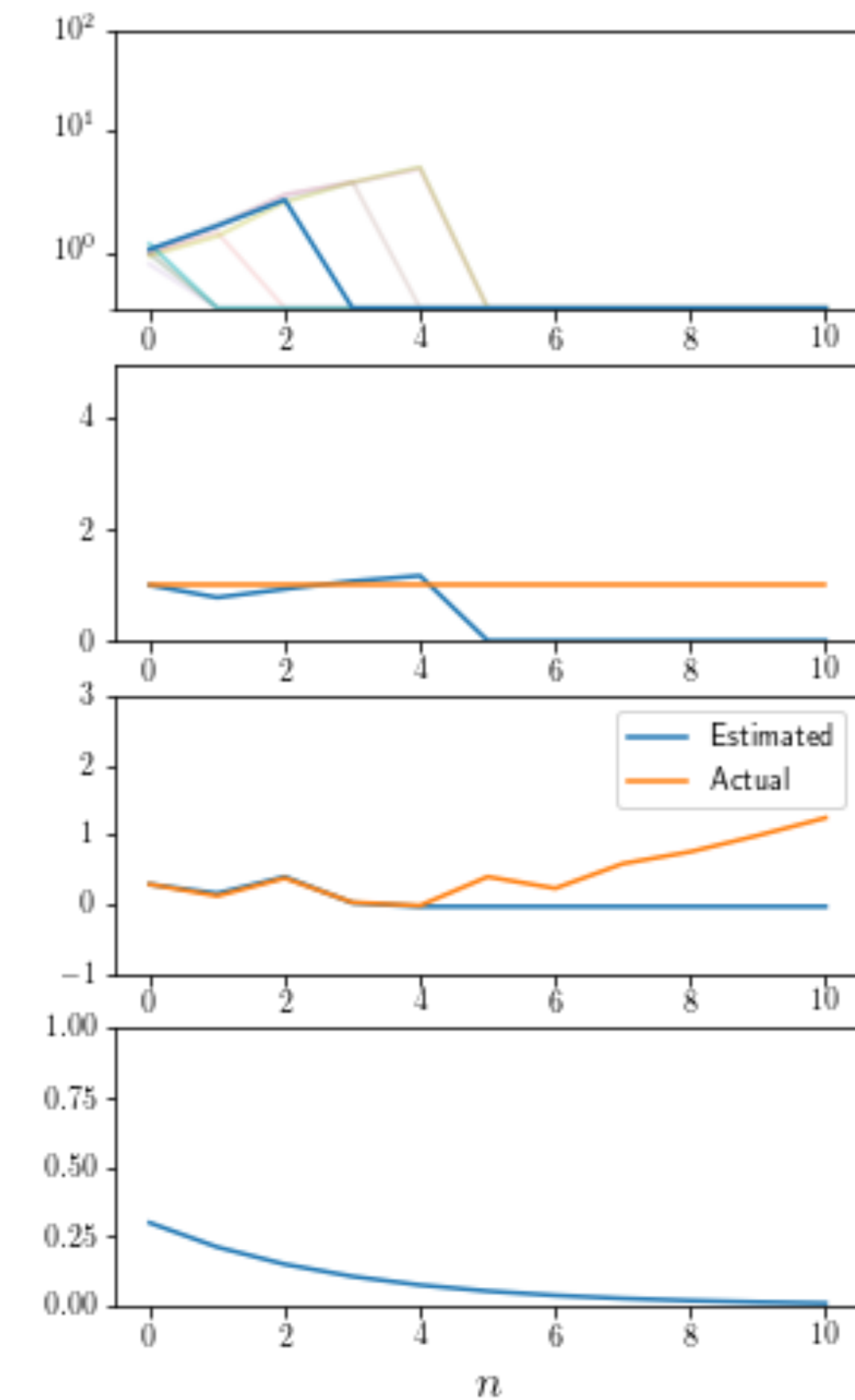
“Single sample”

$$W(n, N) = \frac{1}{q(N)} \mathbb{1}\{n = N\}$$



“Russian roulette”

$$W(n, N) = \frac{1}{1 - \sum_{n'=1}^{n-1} q(n')} \mathbb{1}\{N \geq n\}$$





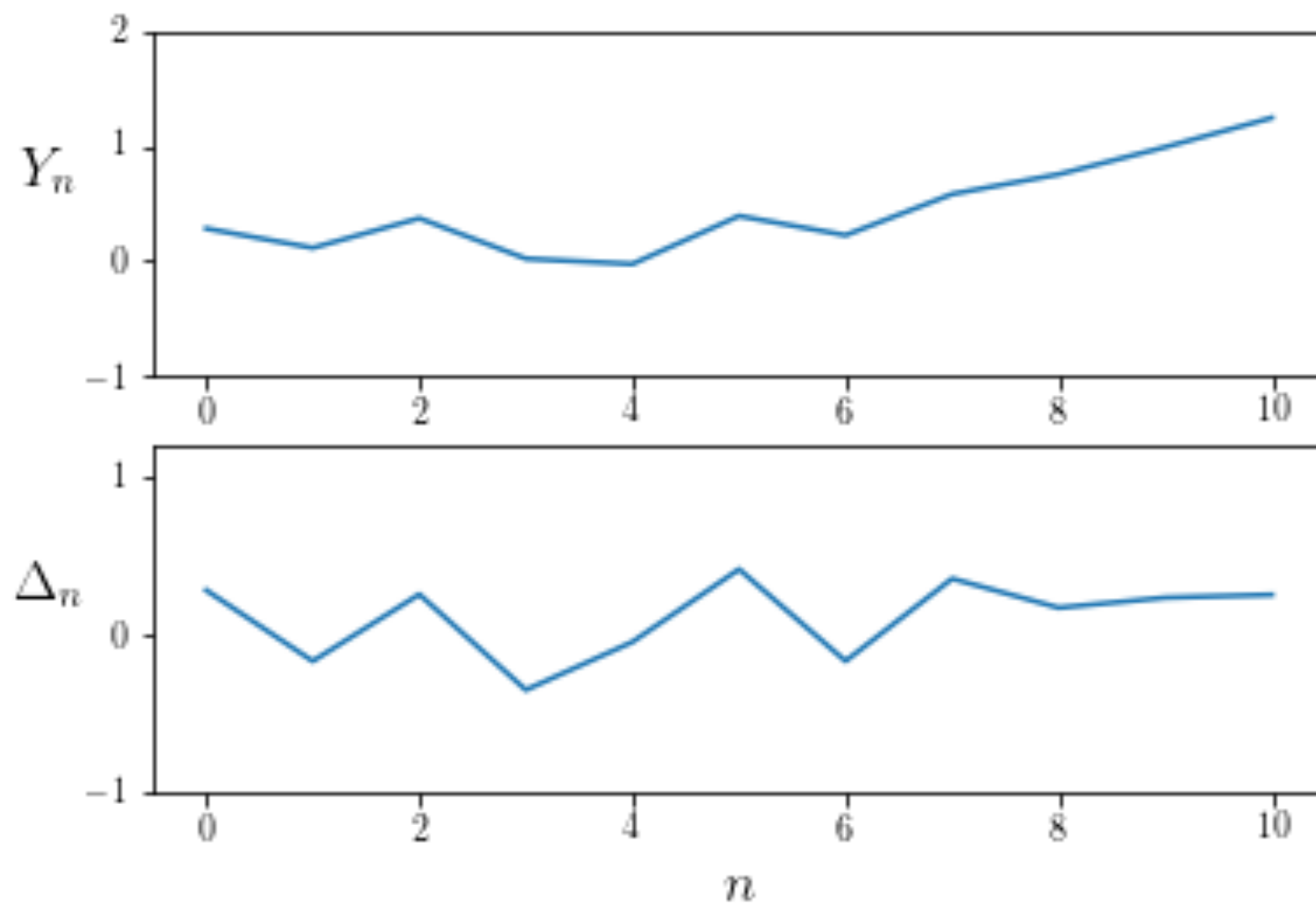
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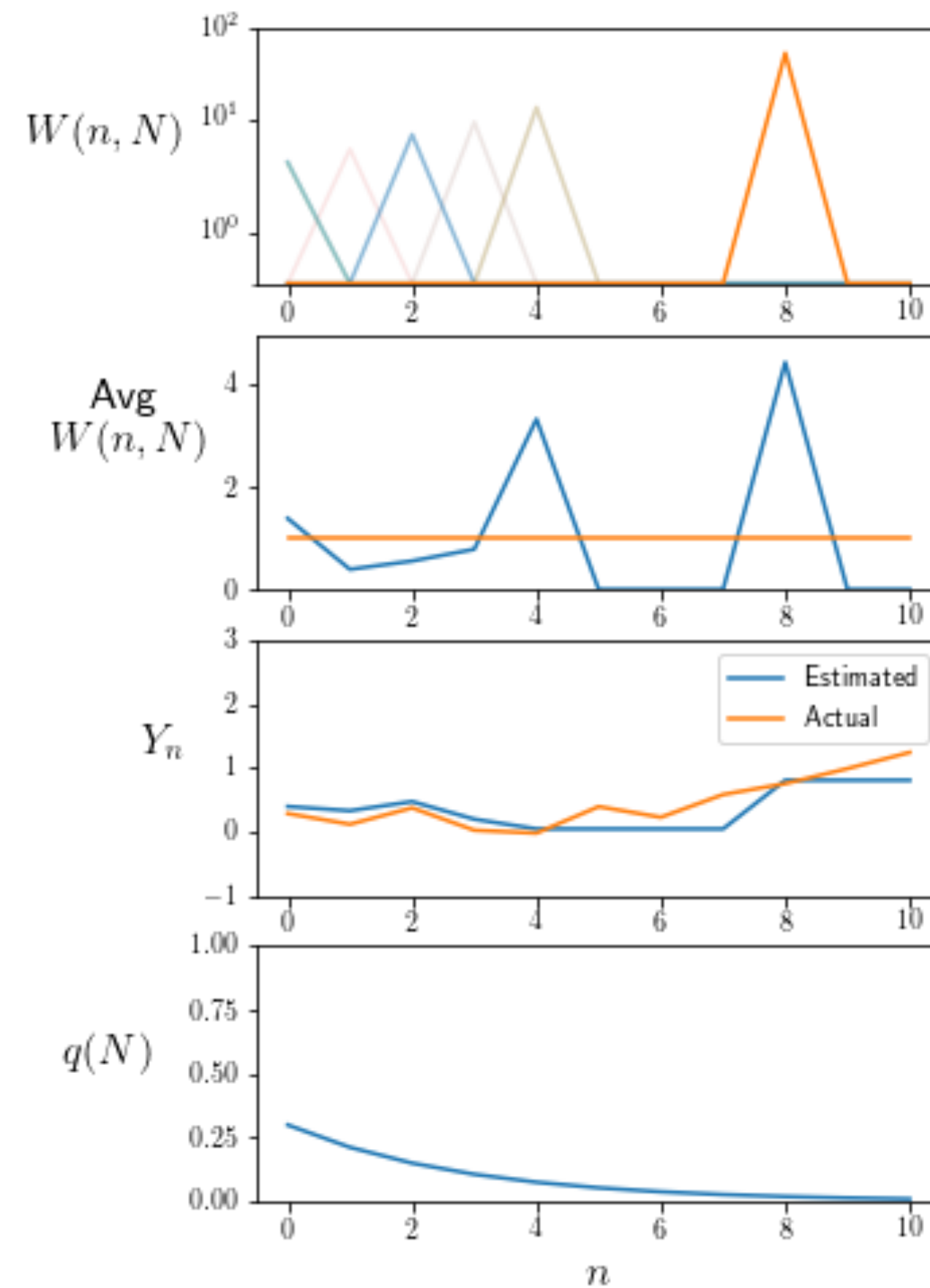
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Ground truth



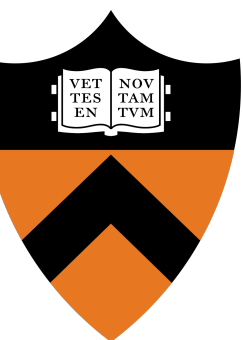
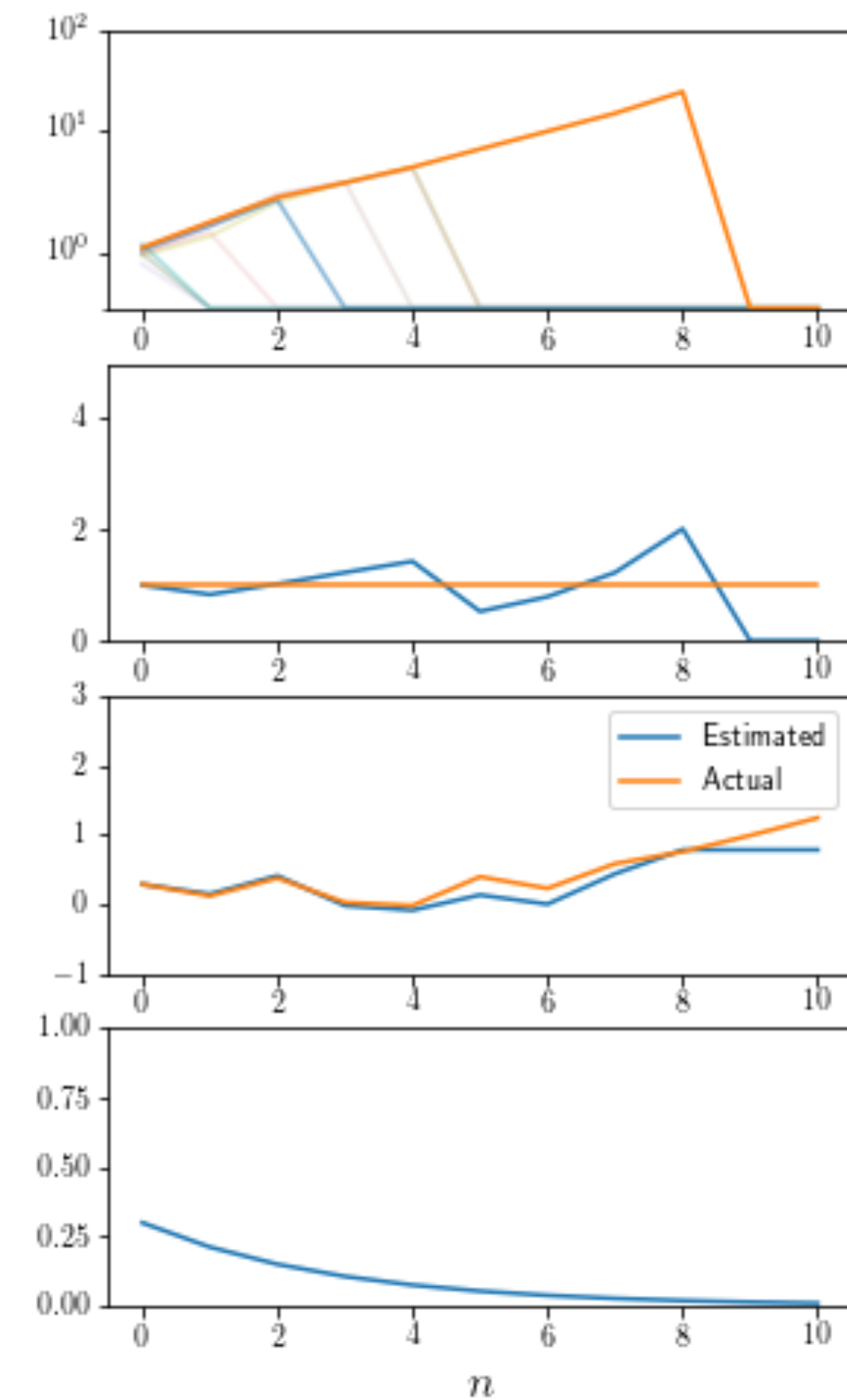
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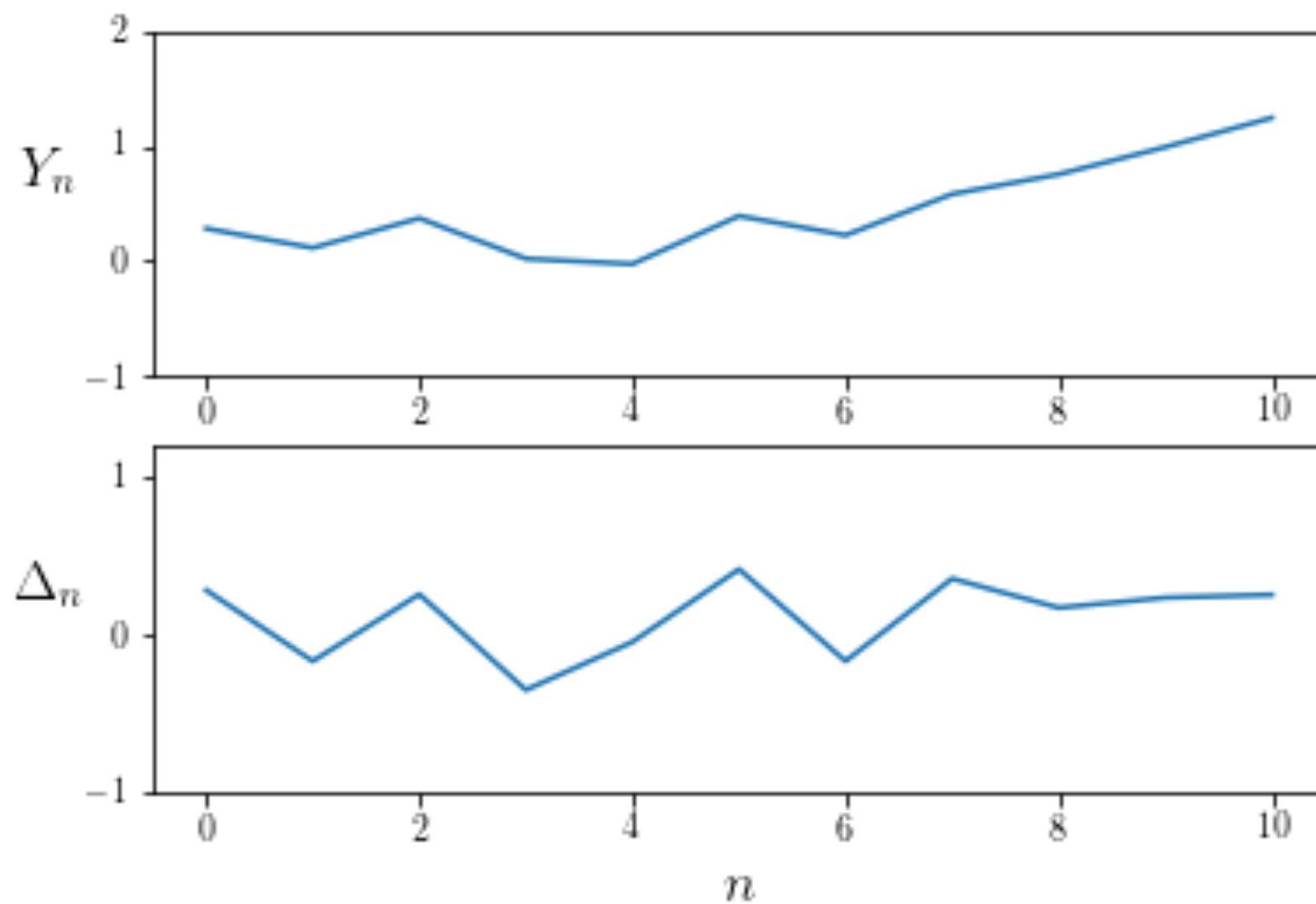
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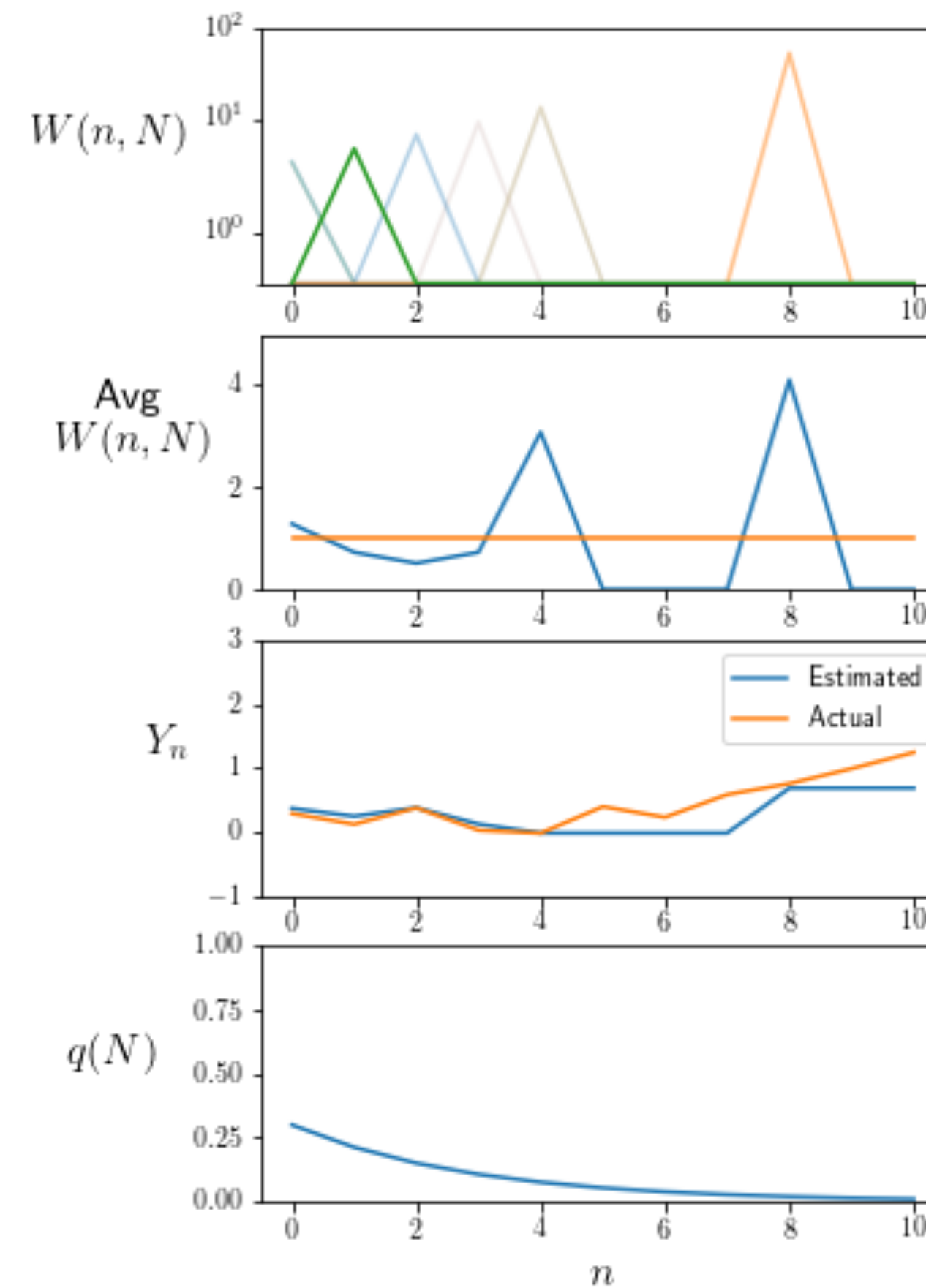
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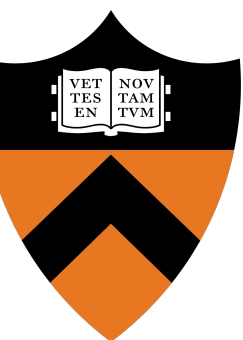
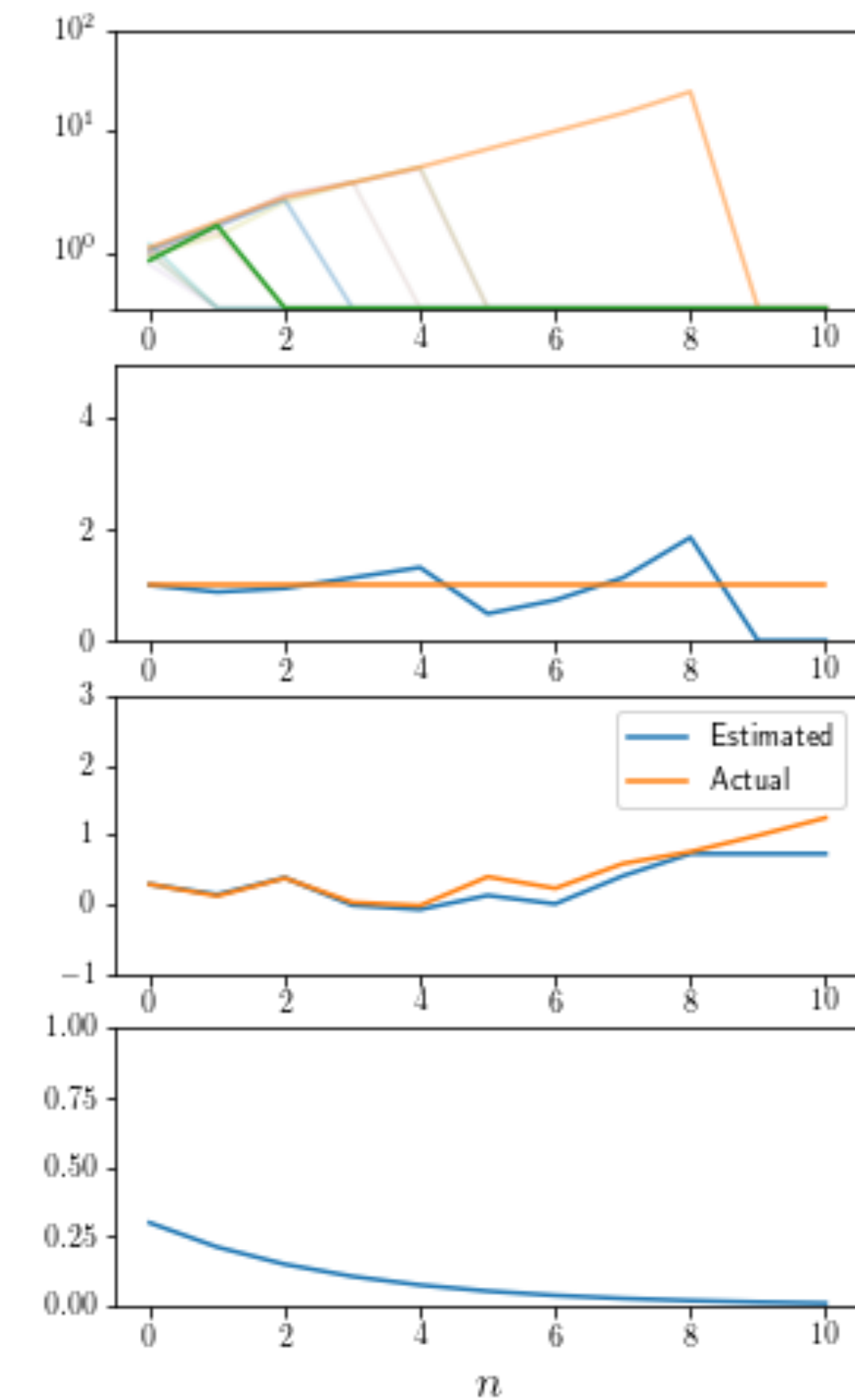
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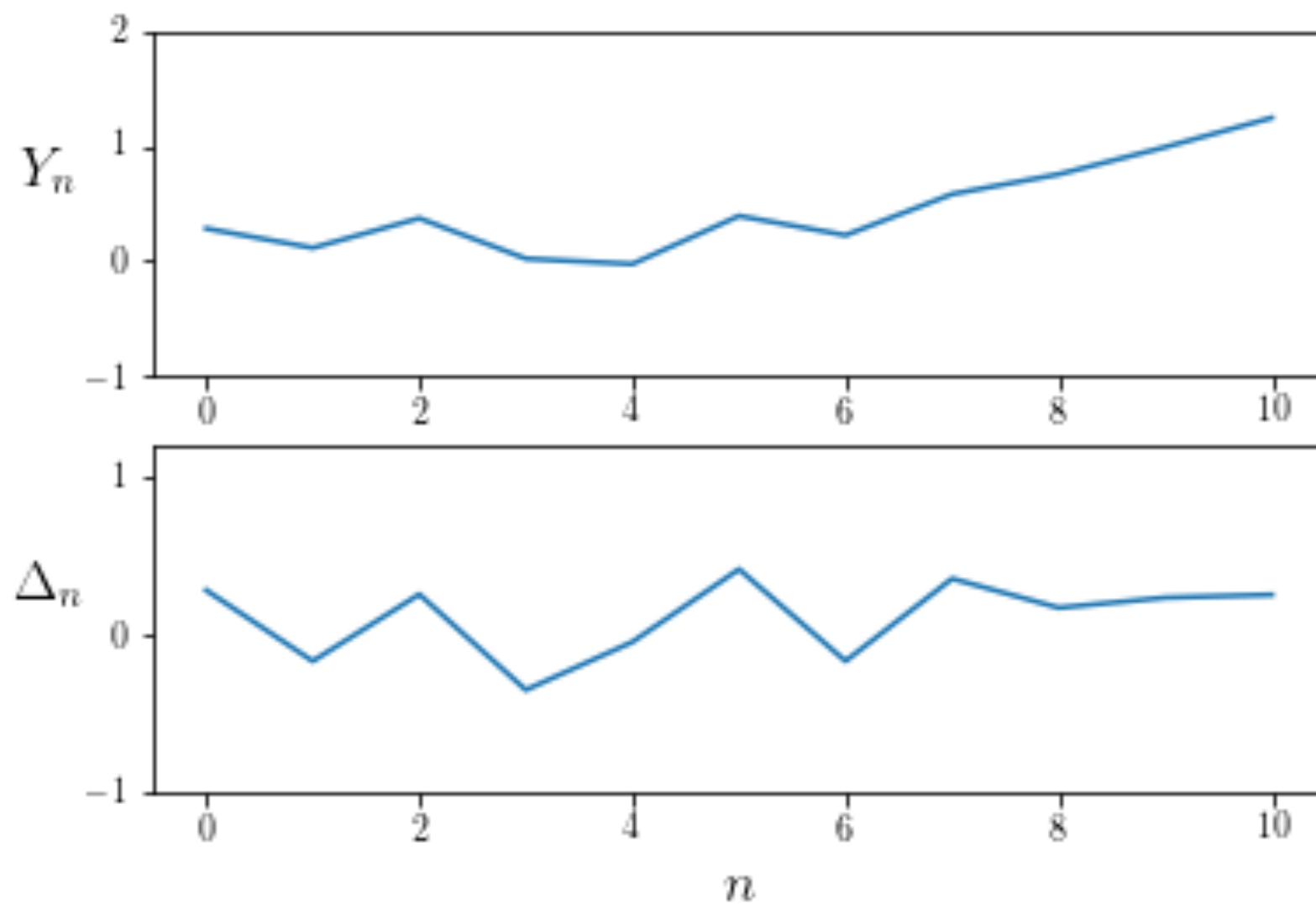
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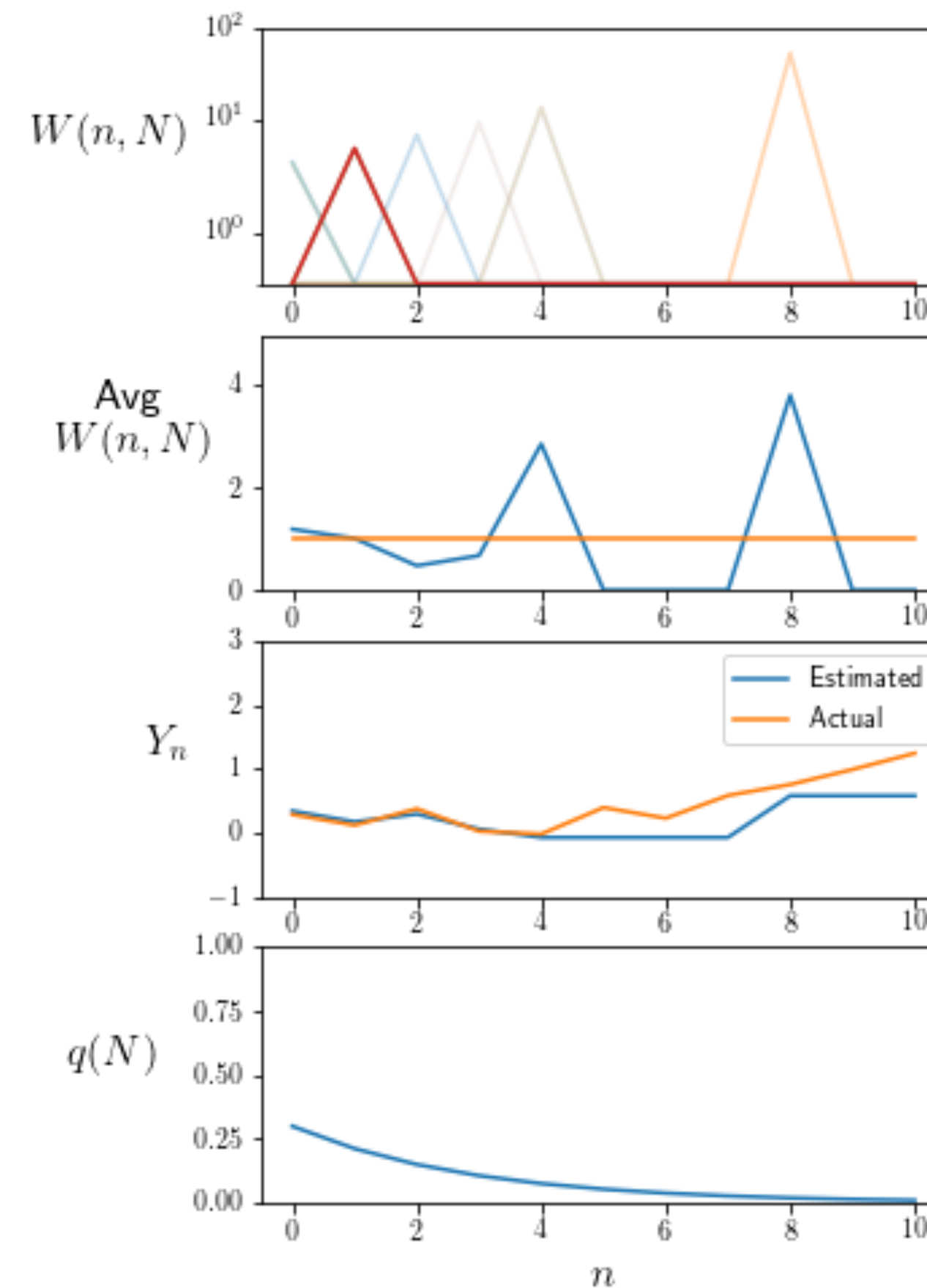
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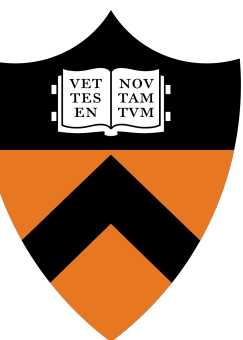
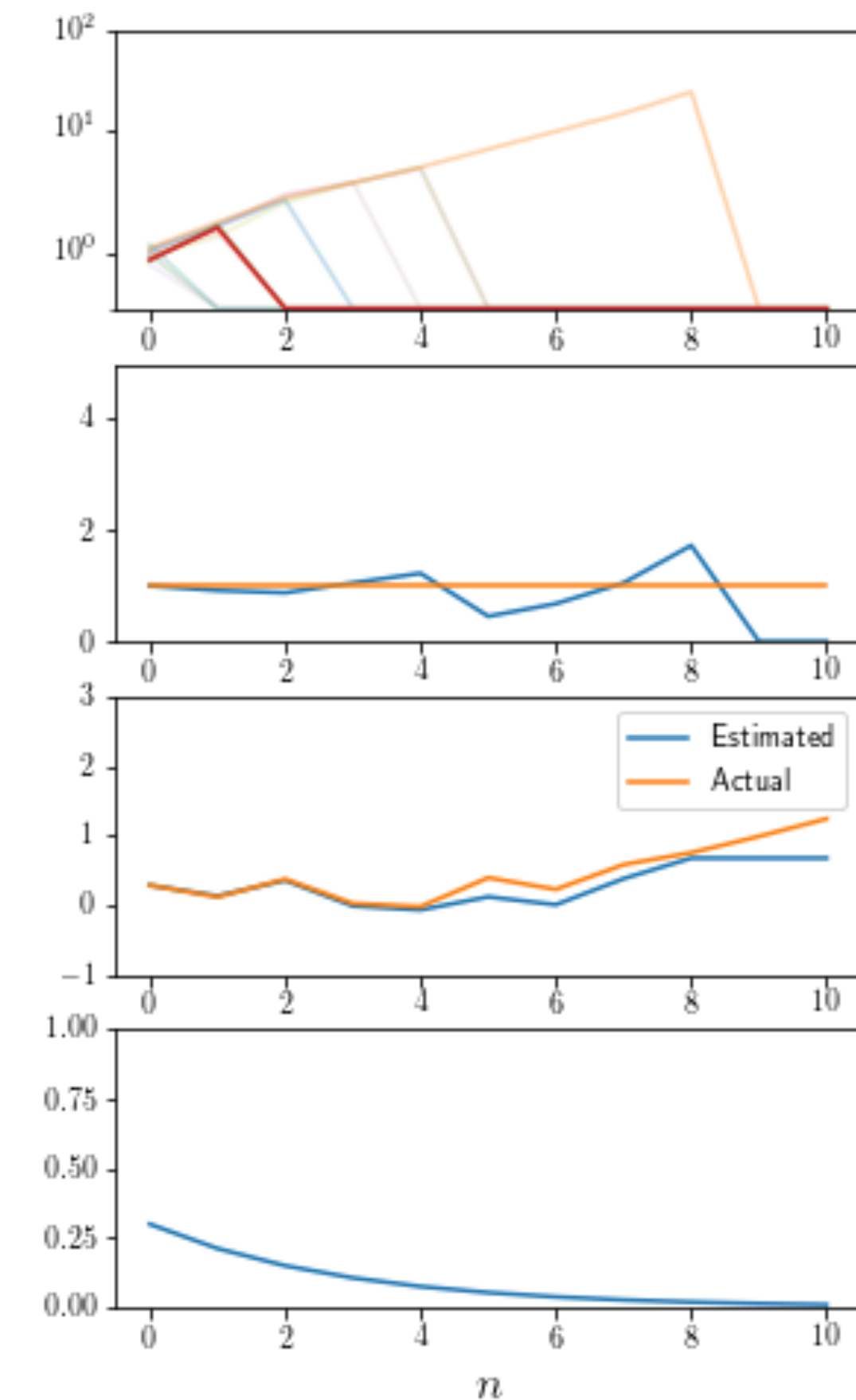
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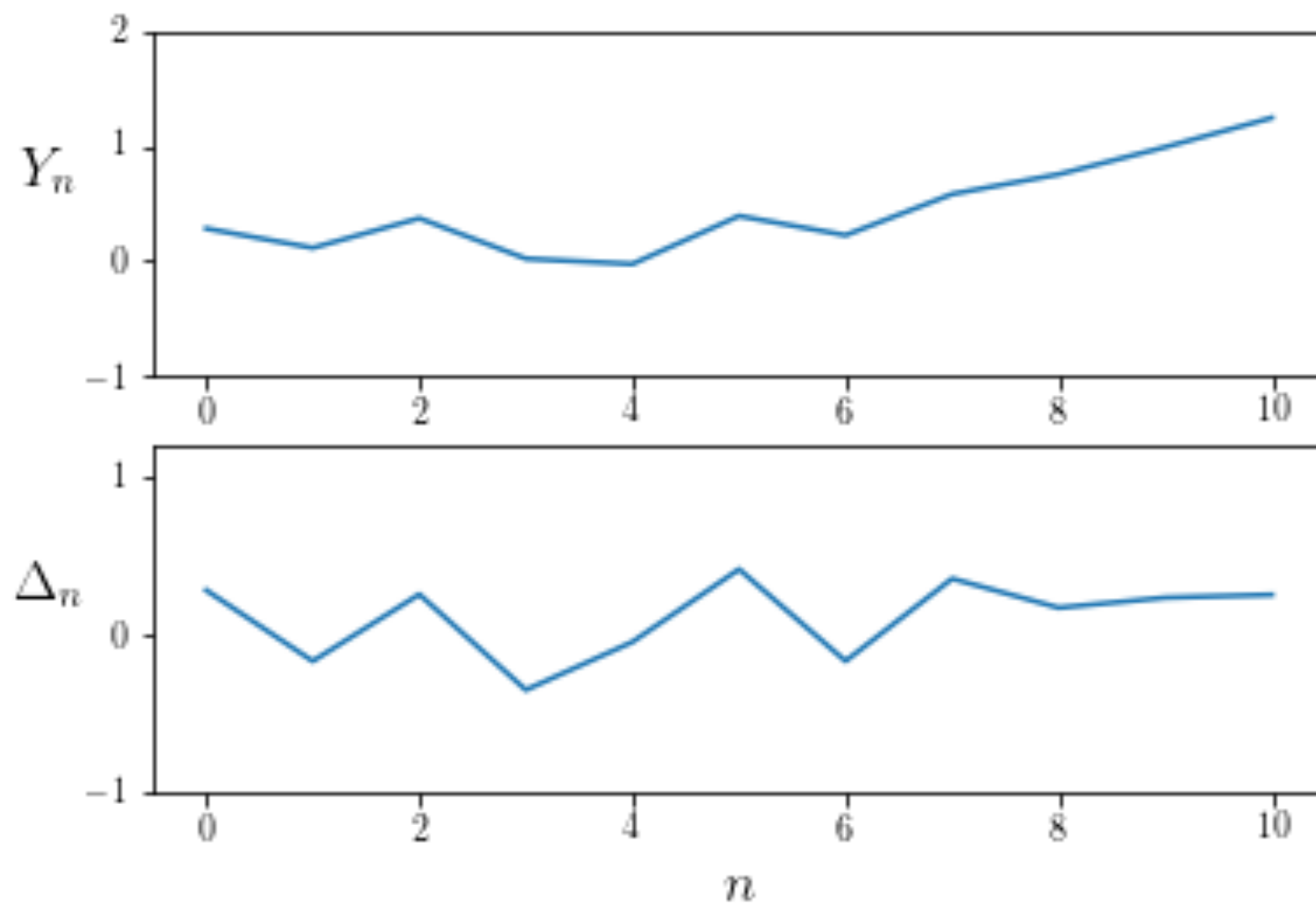
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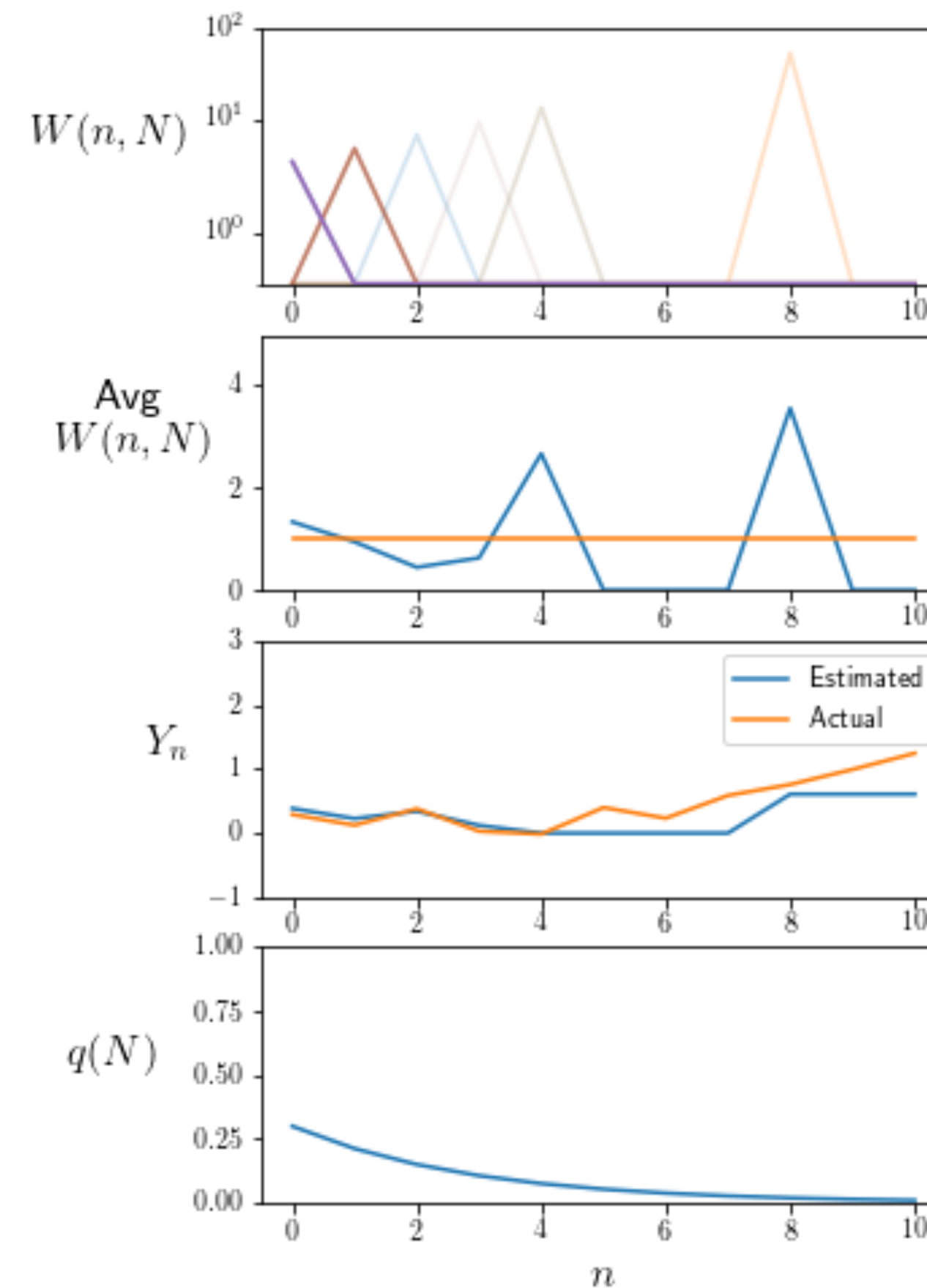
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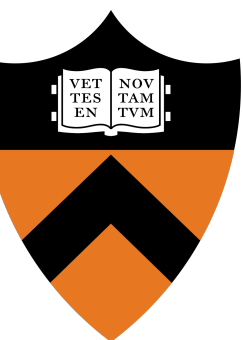
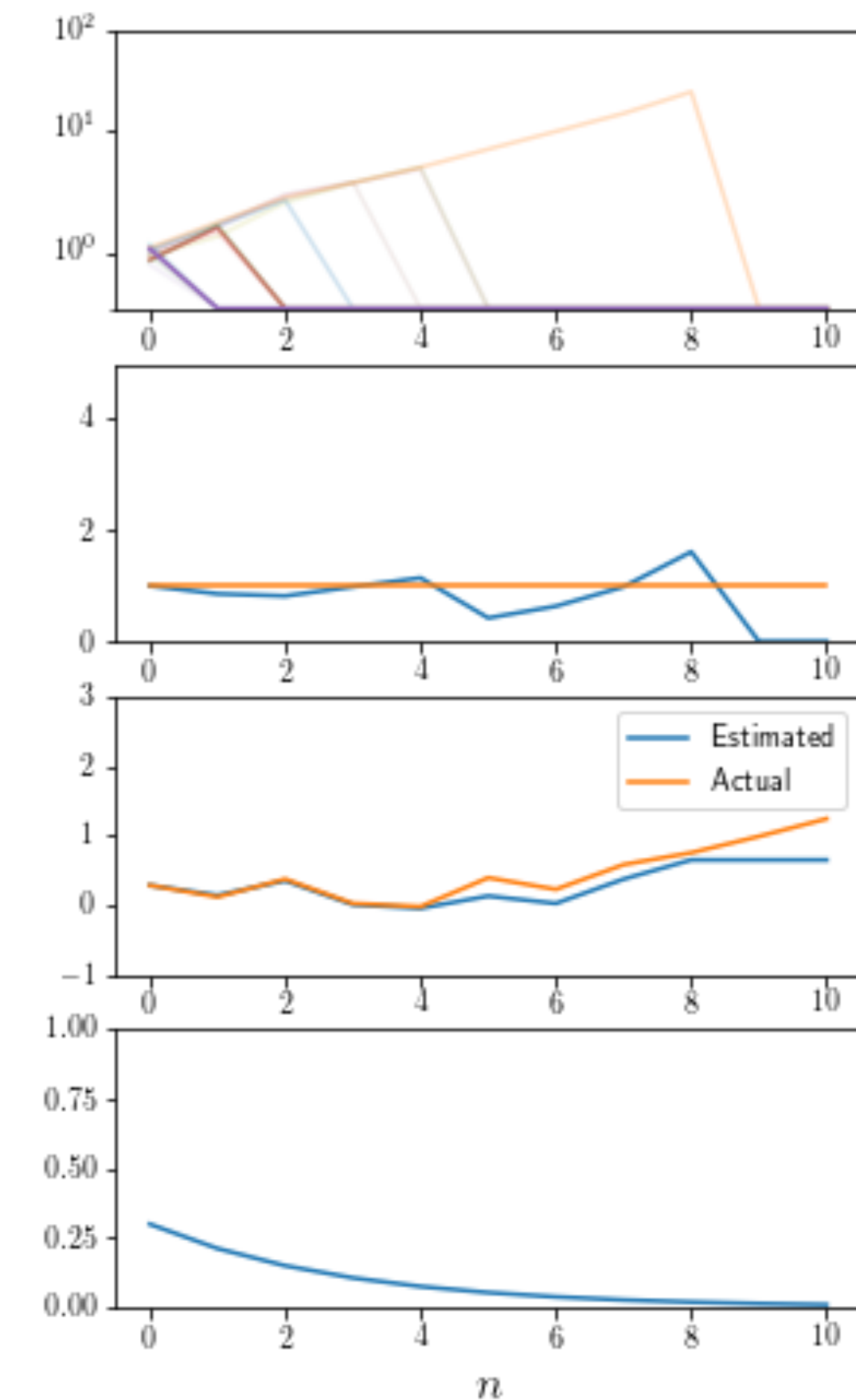
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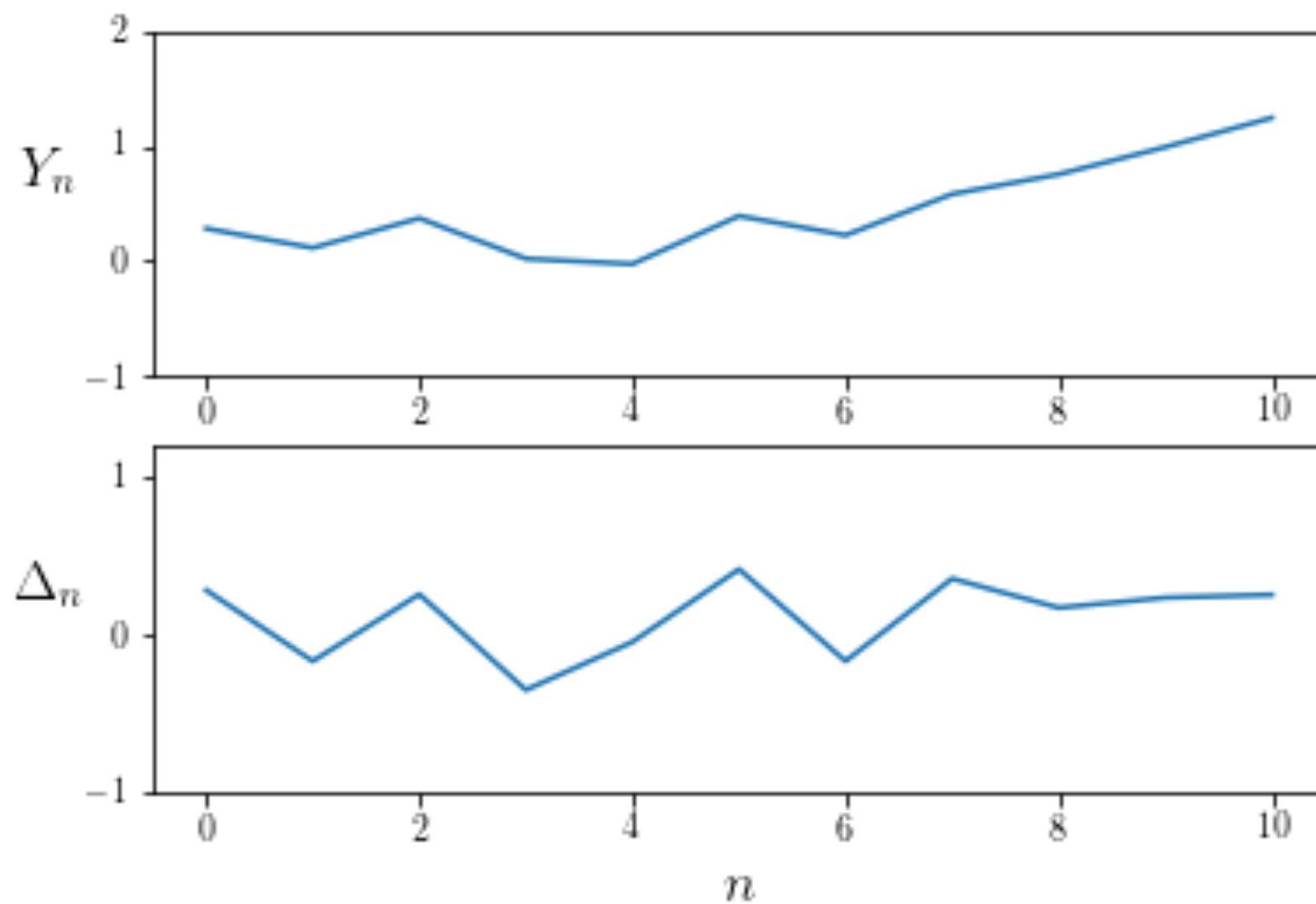
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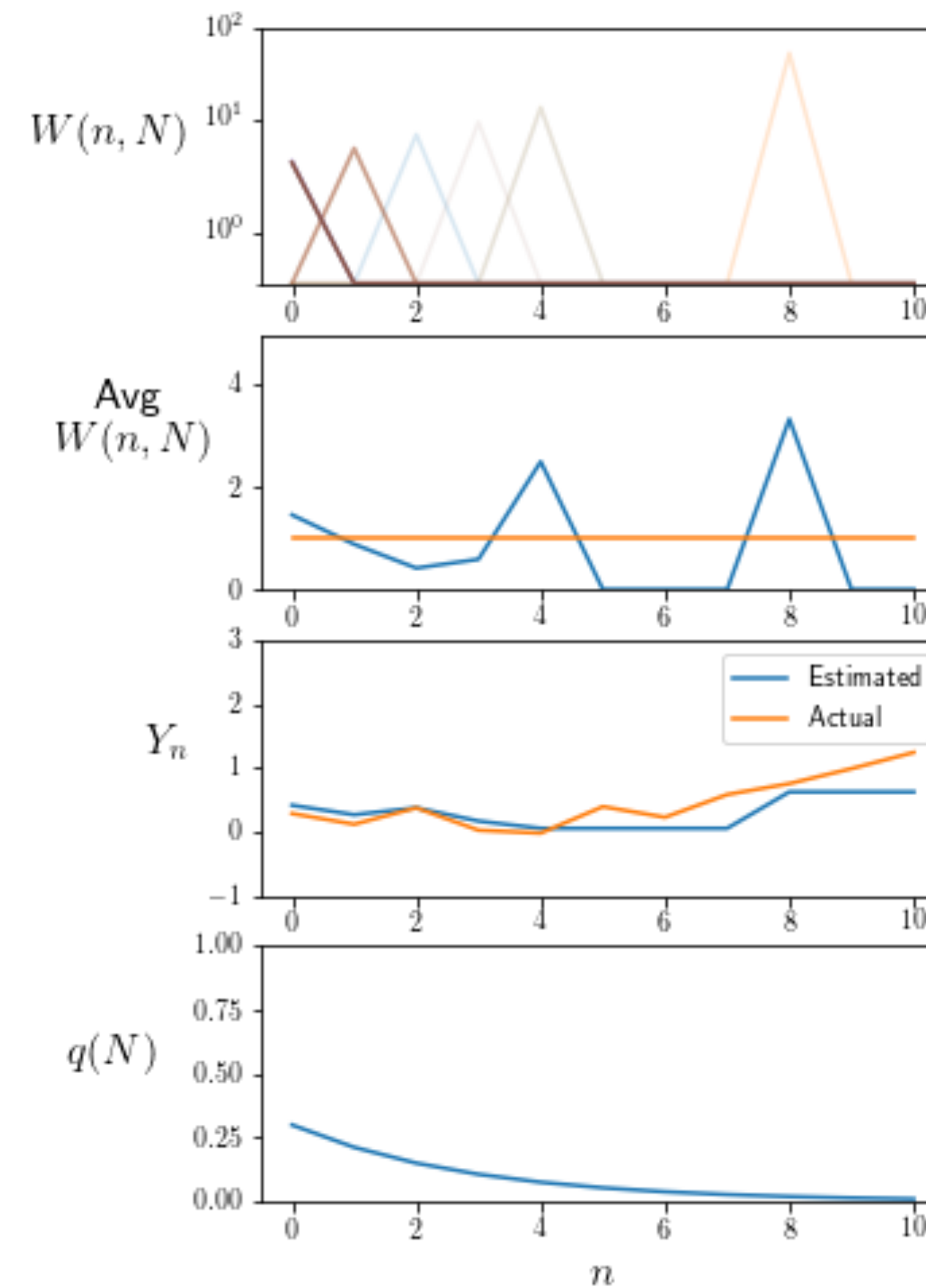
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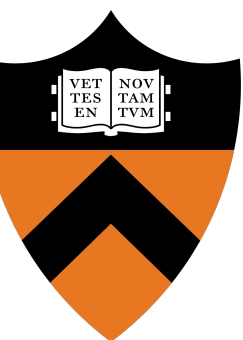
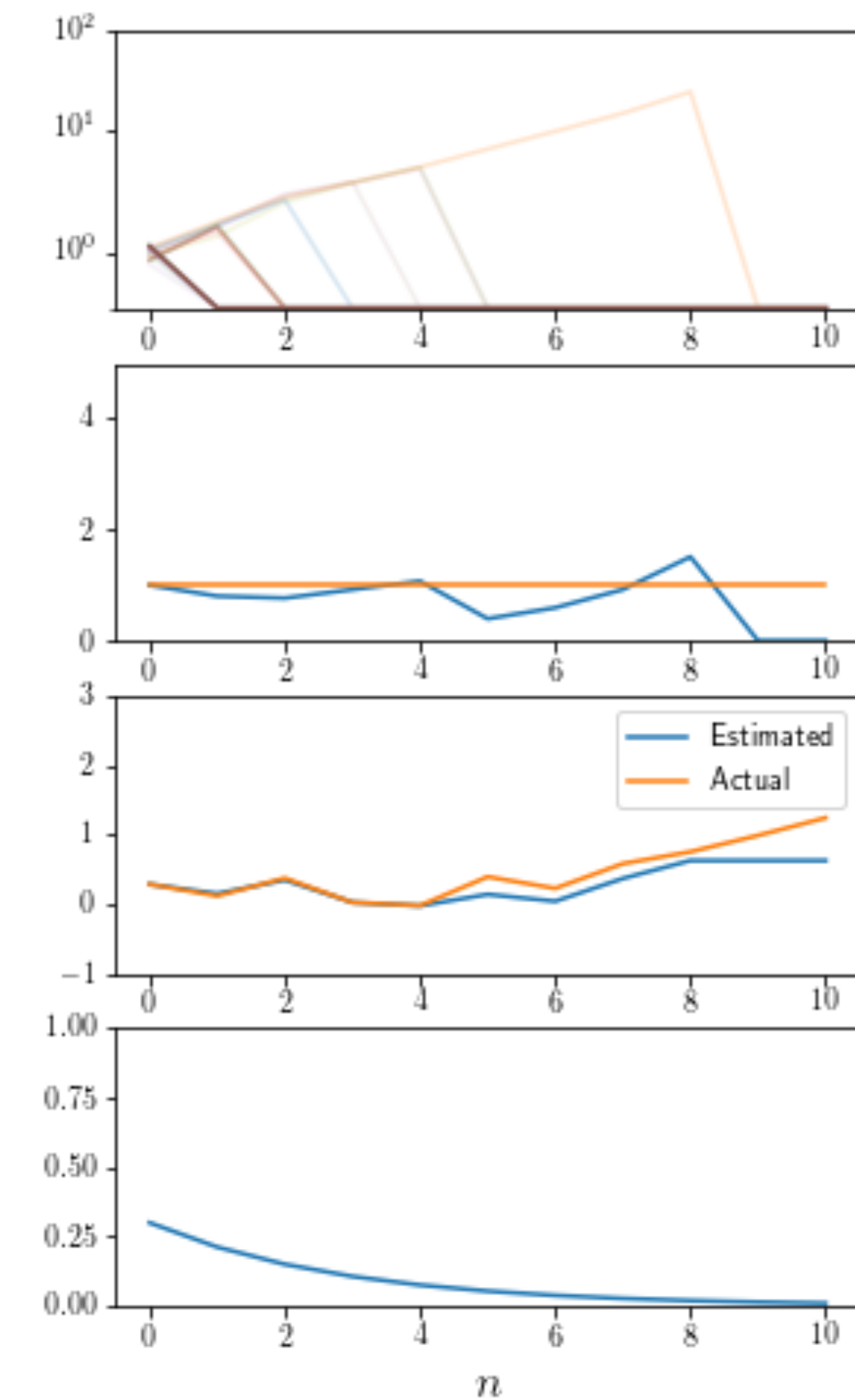
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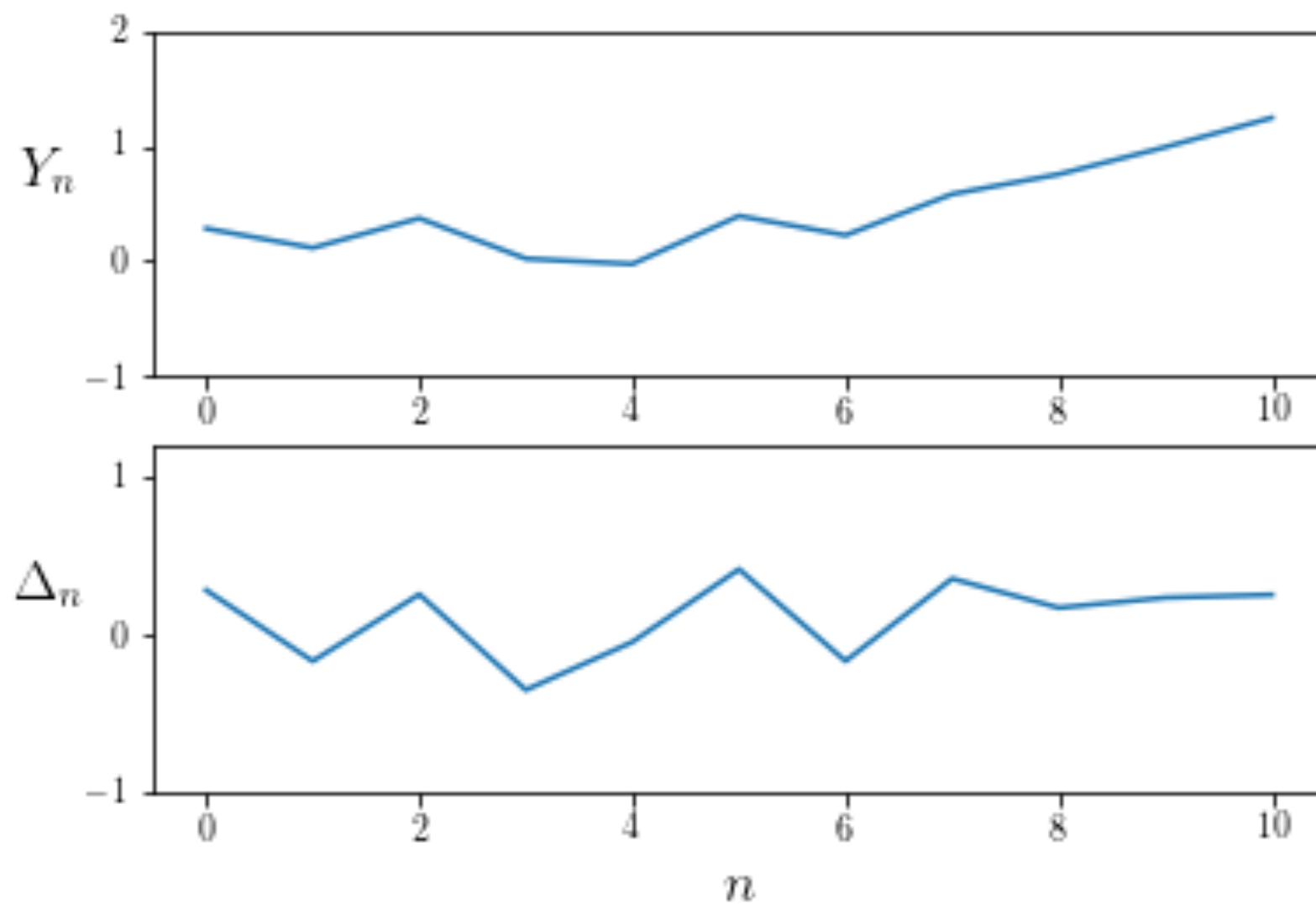
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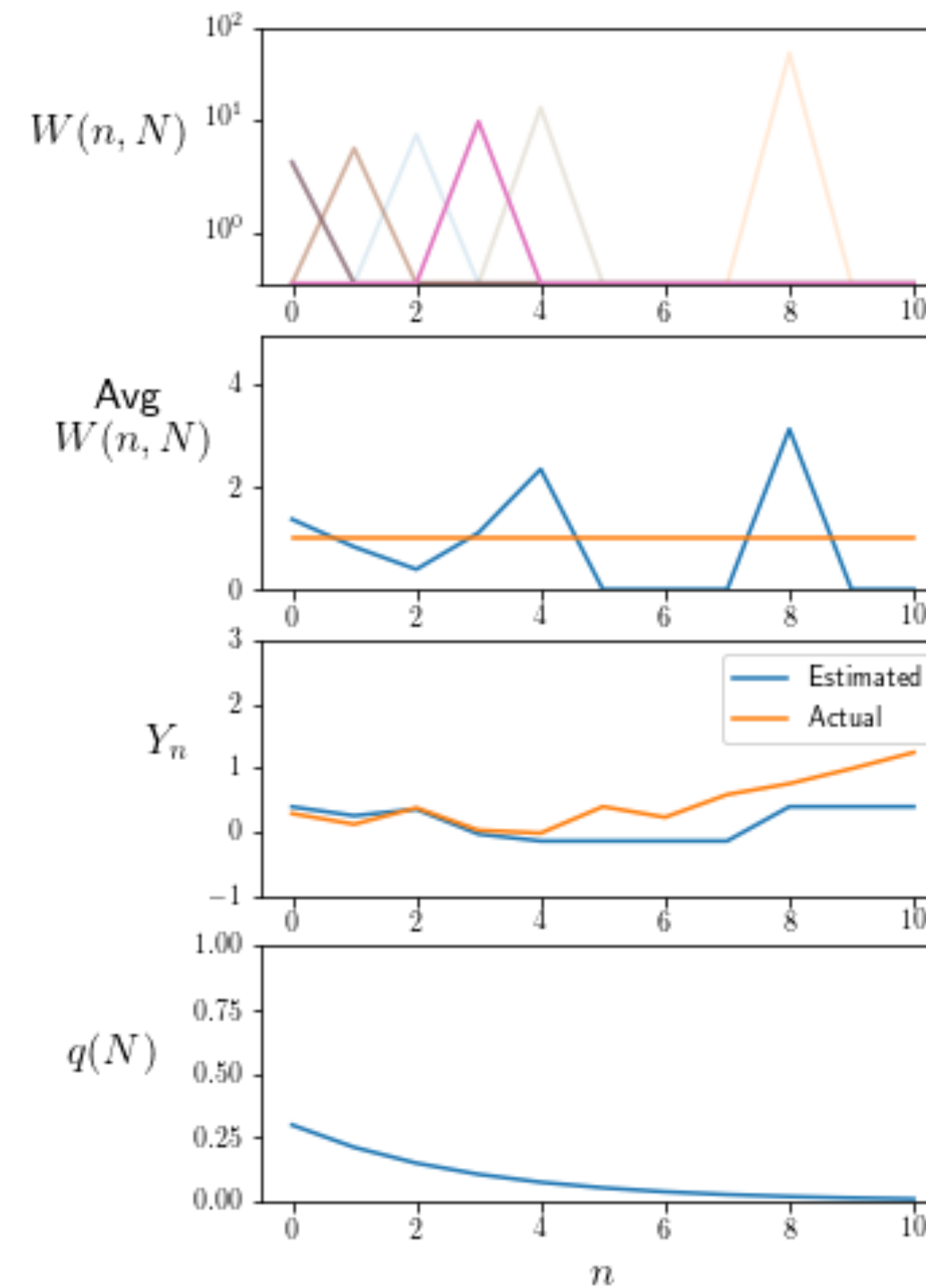
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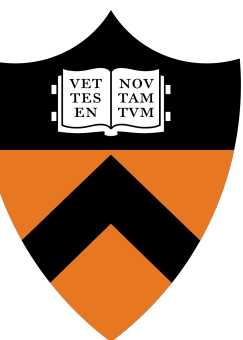
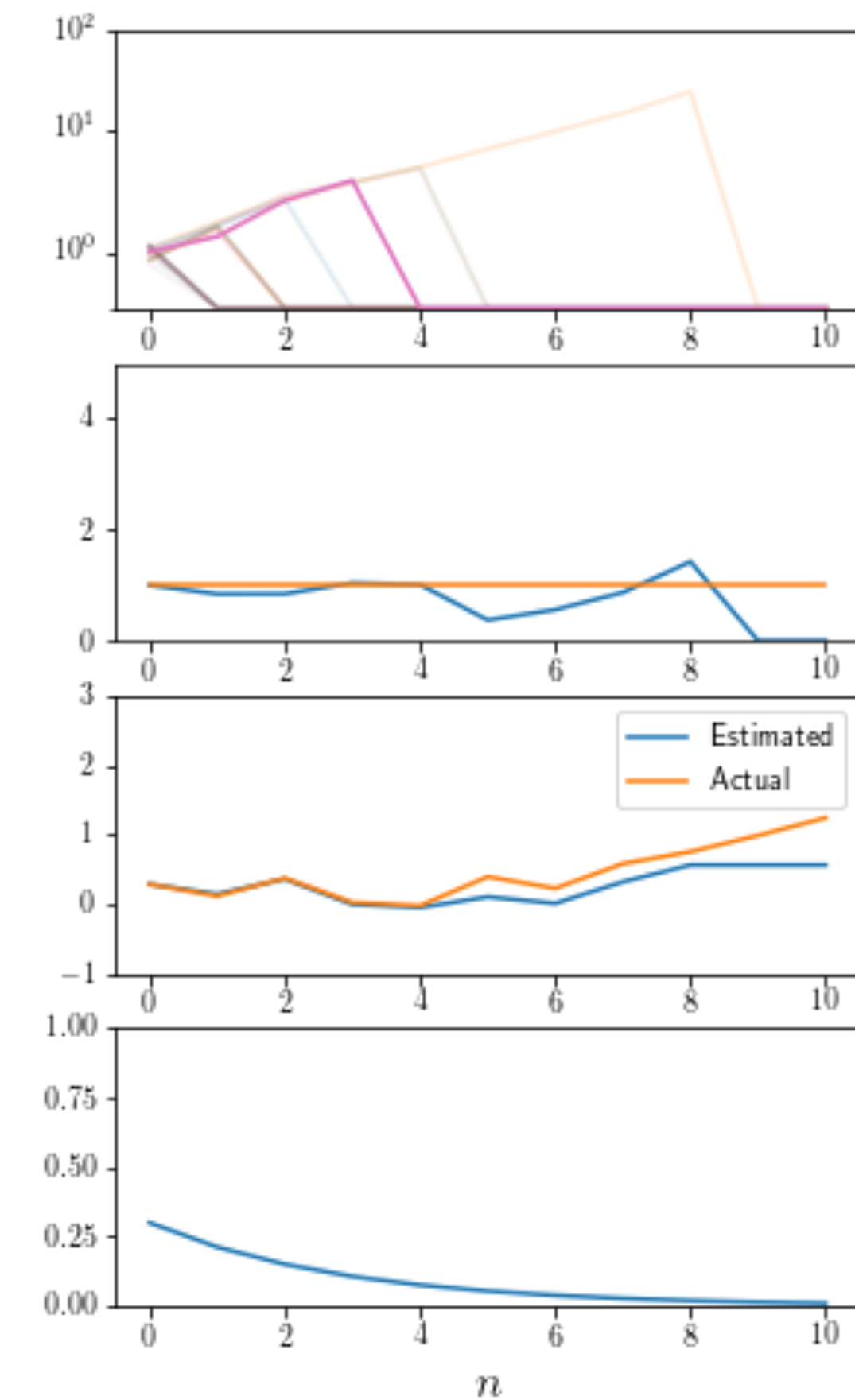
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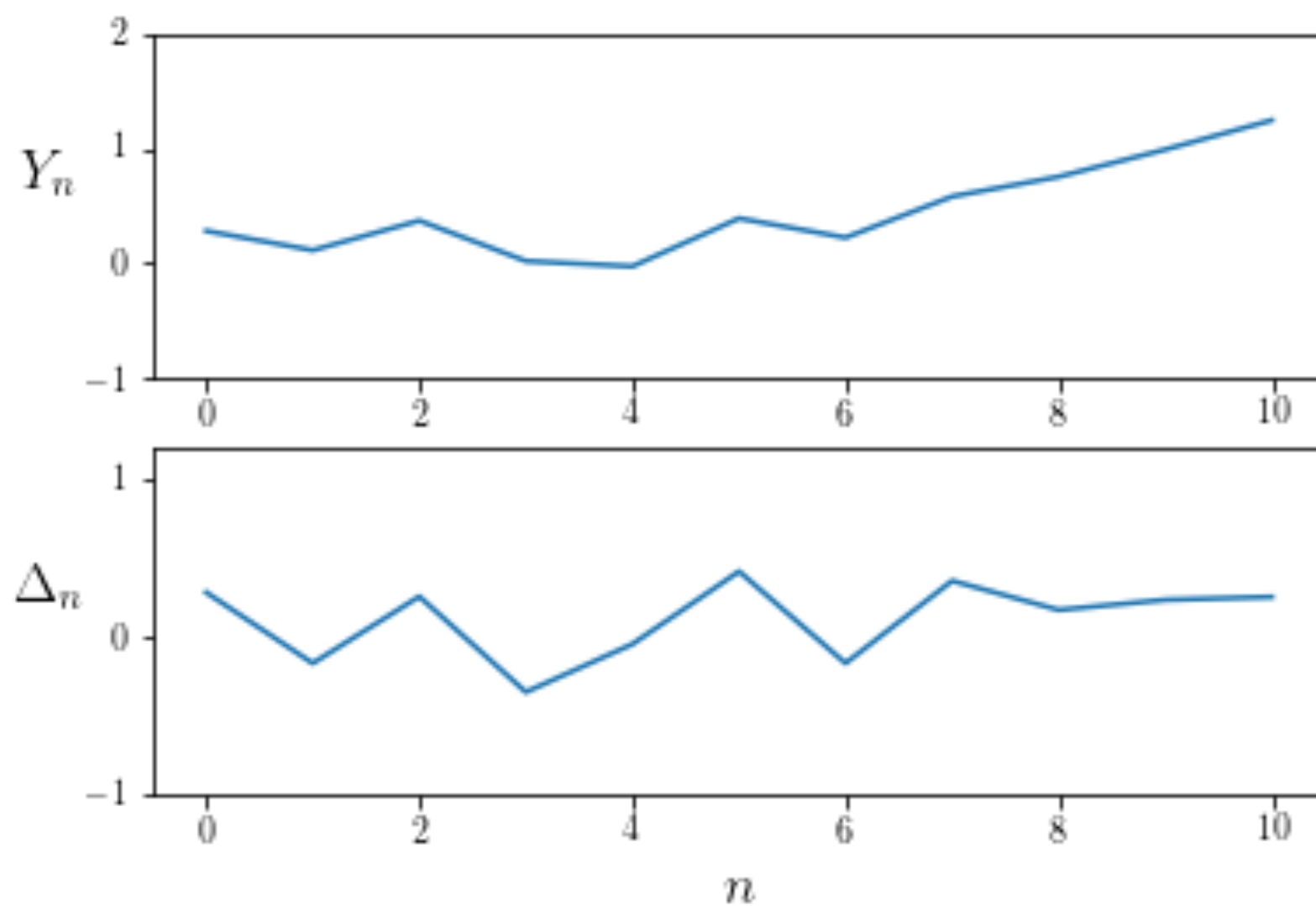
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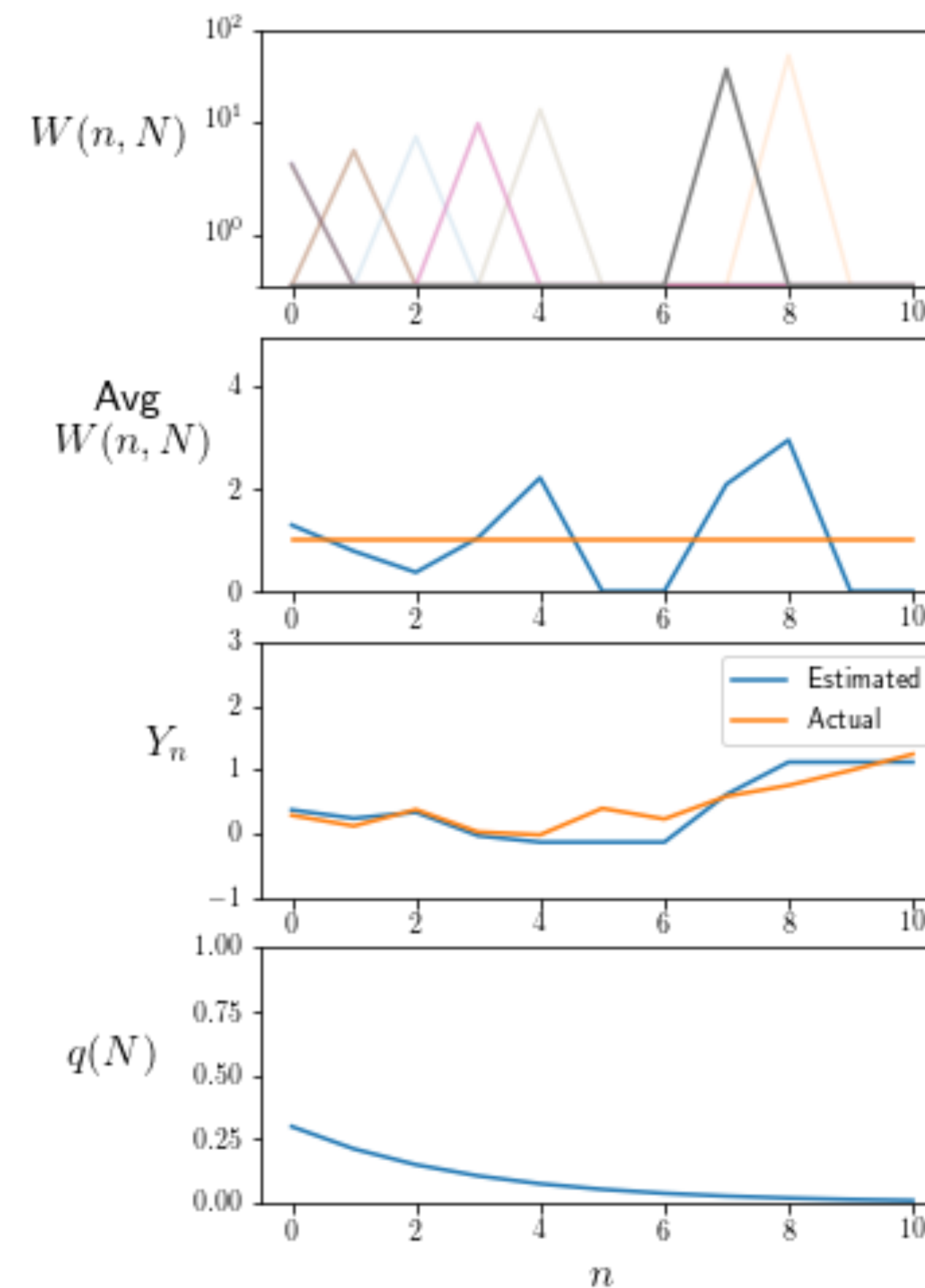
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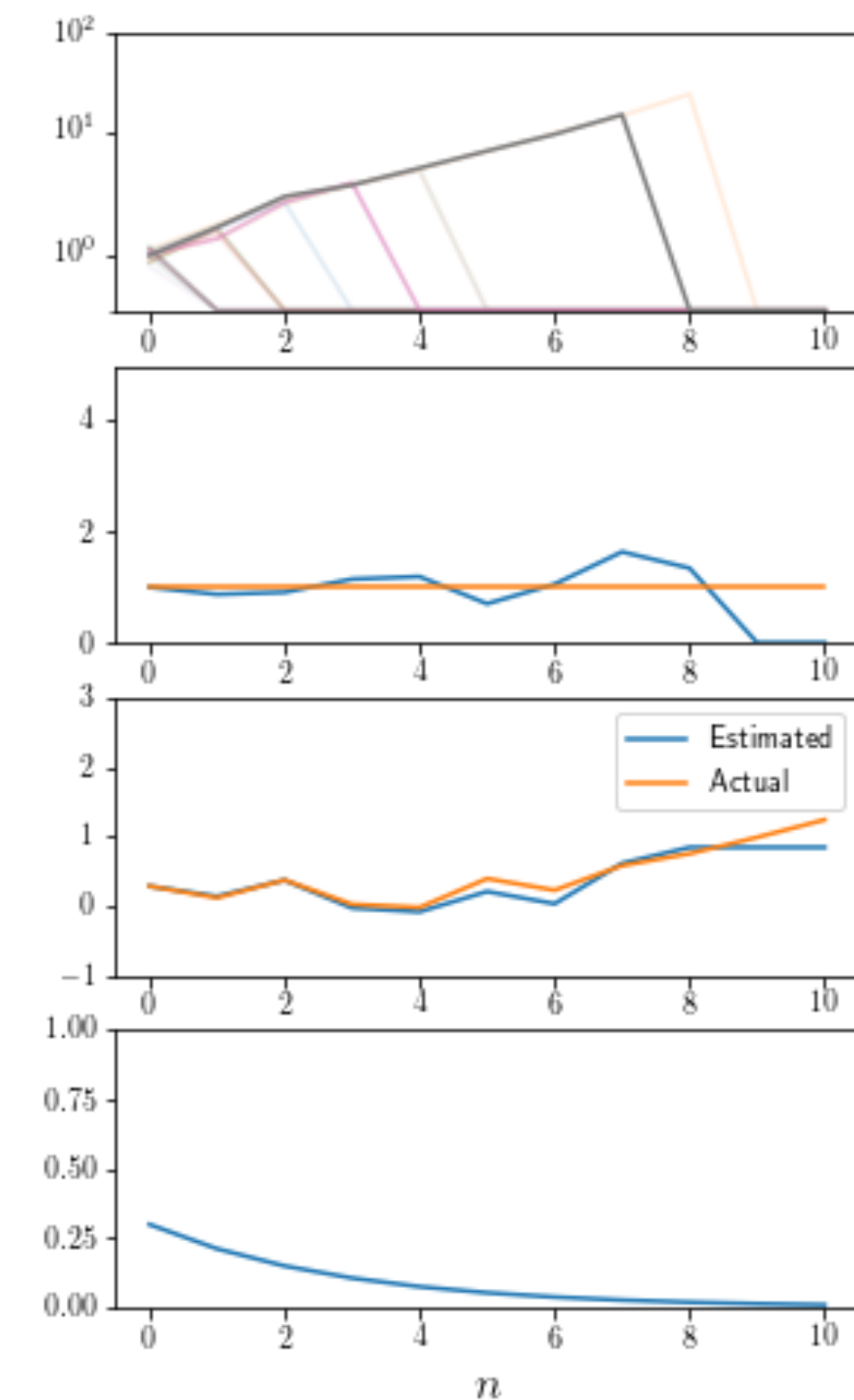
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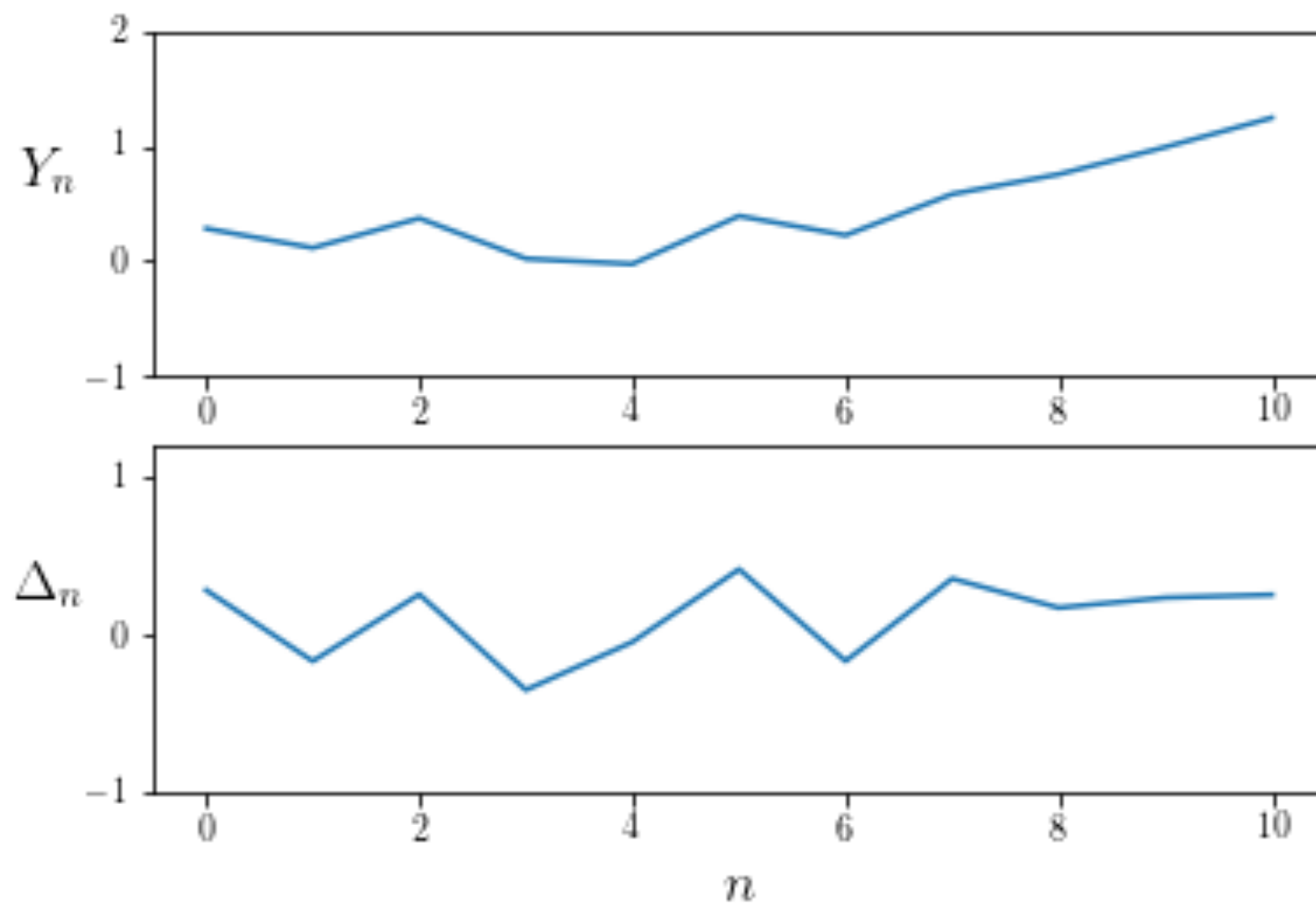
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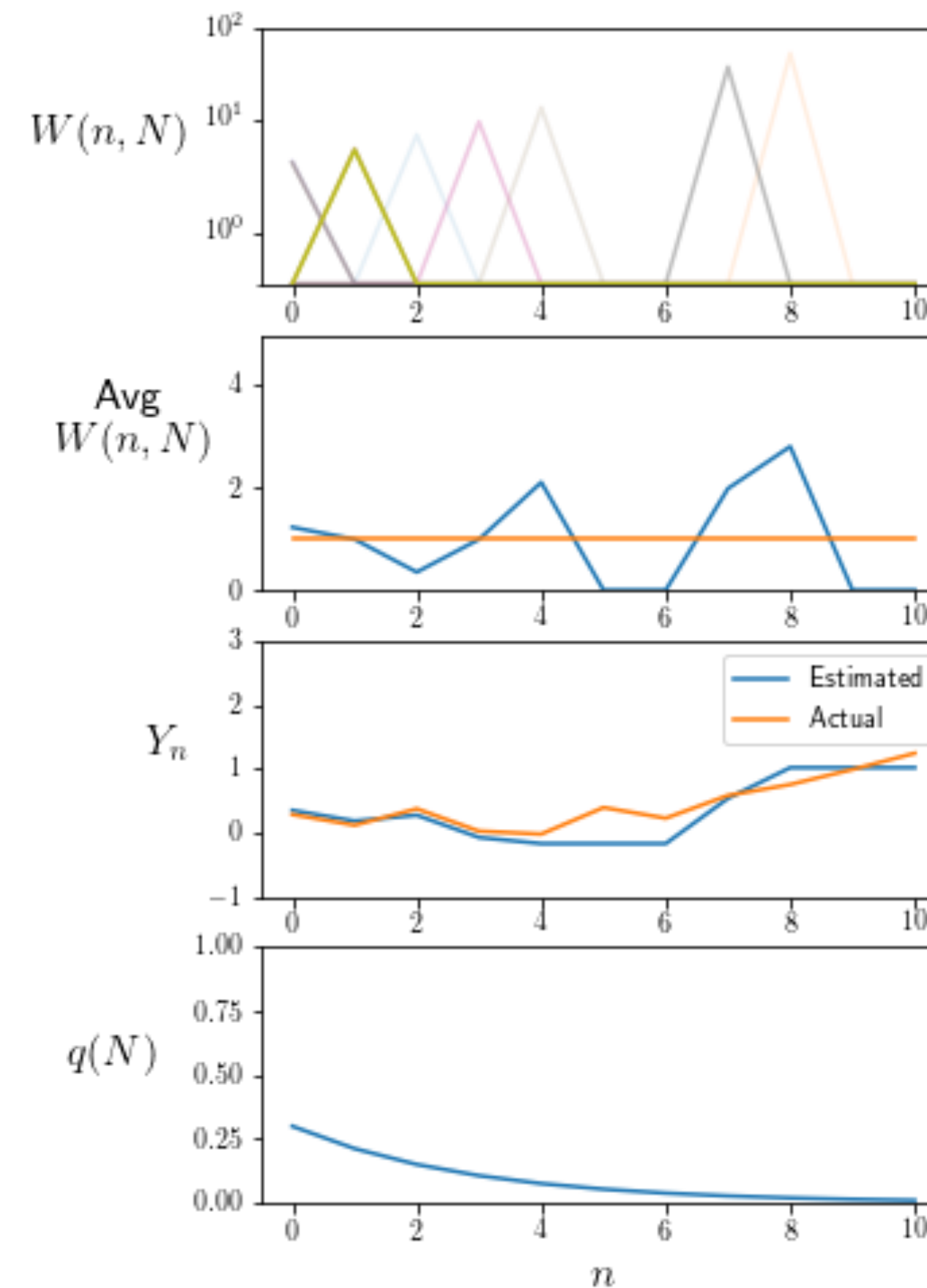
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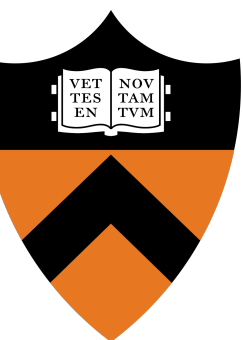
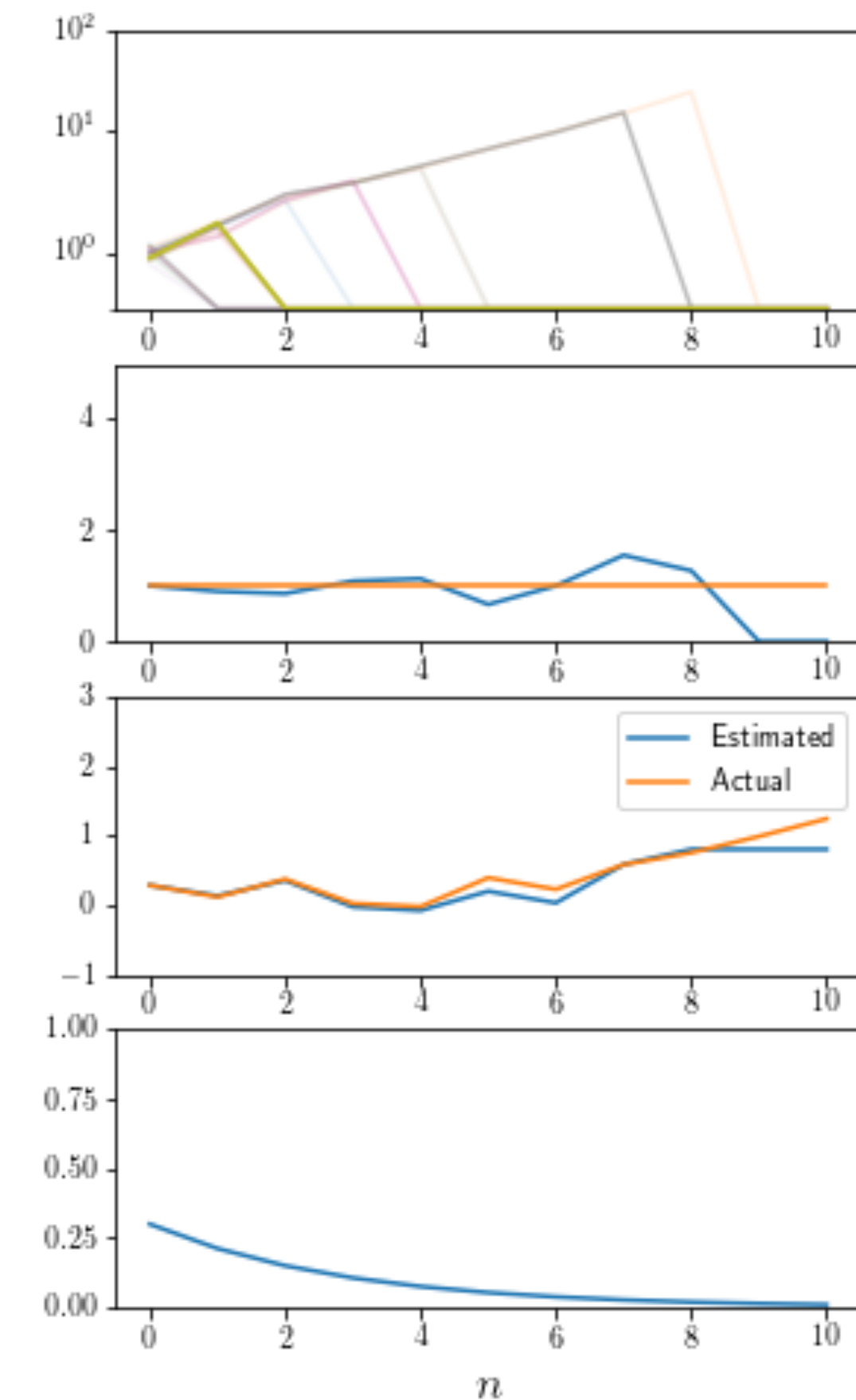
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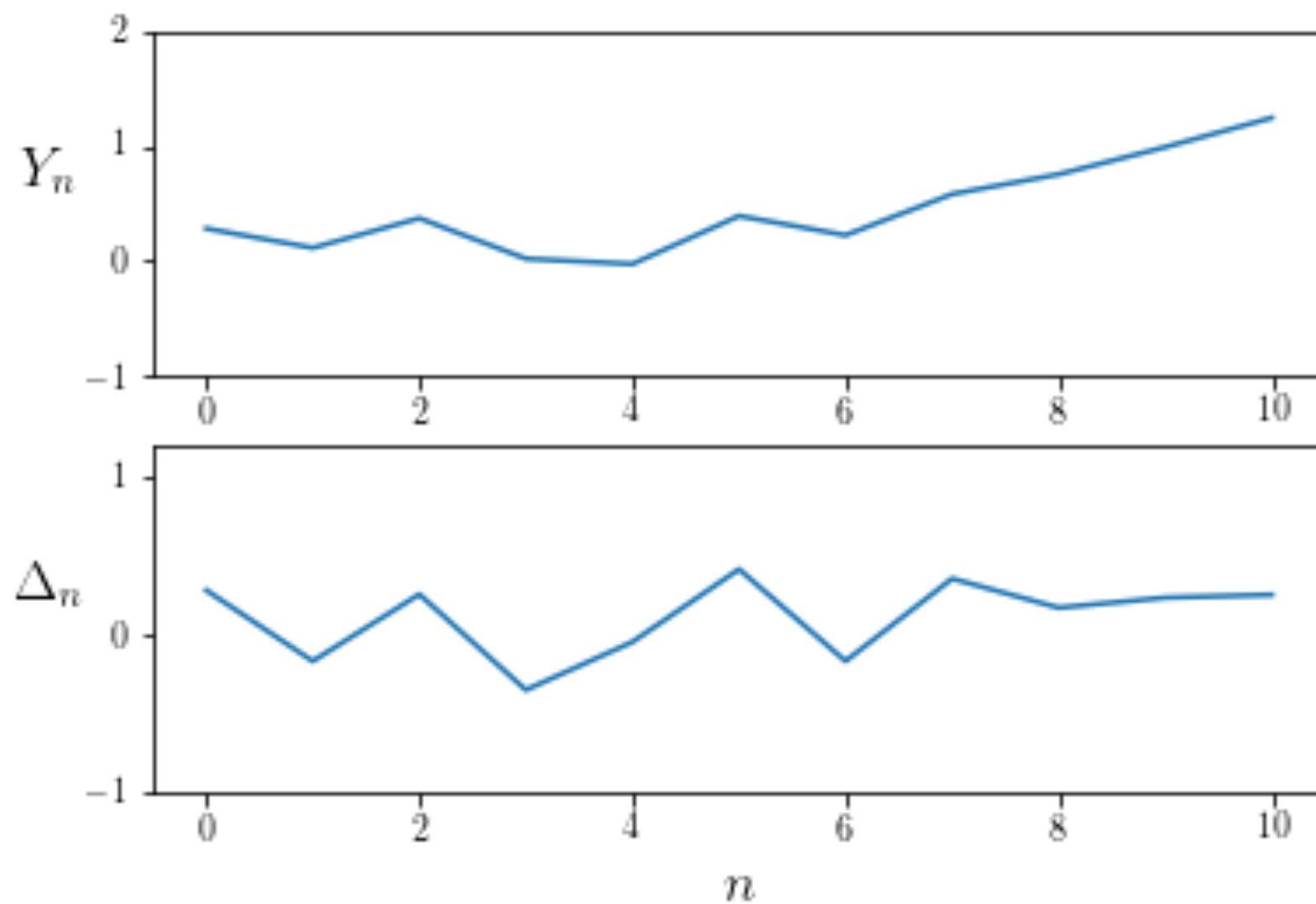
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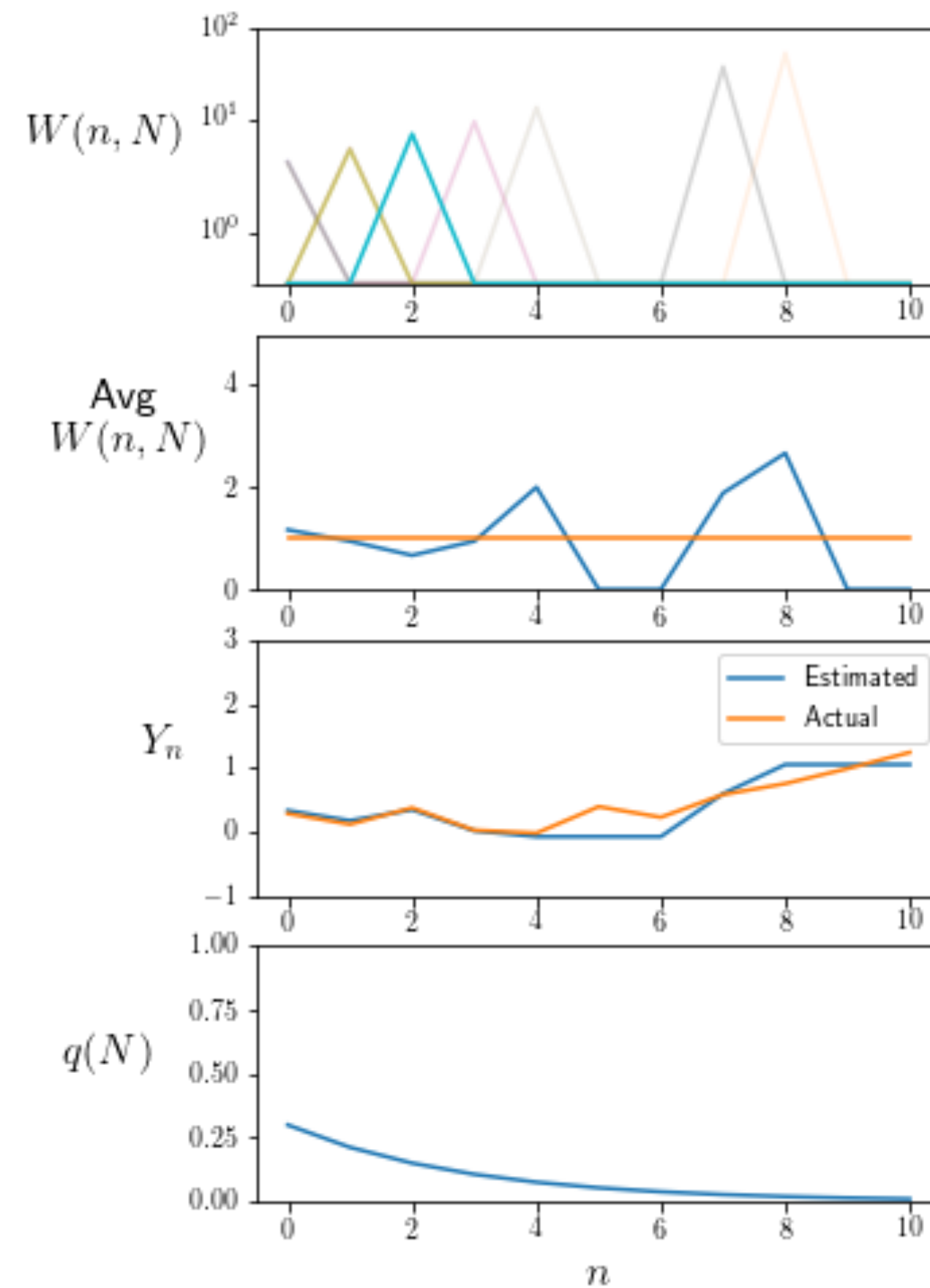
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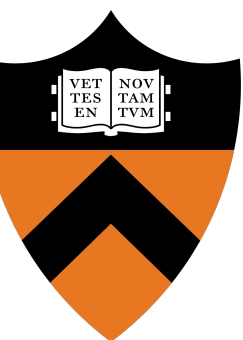
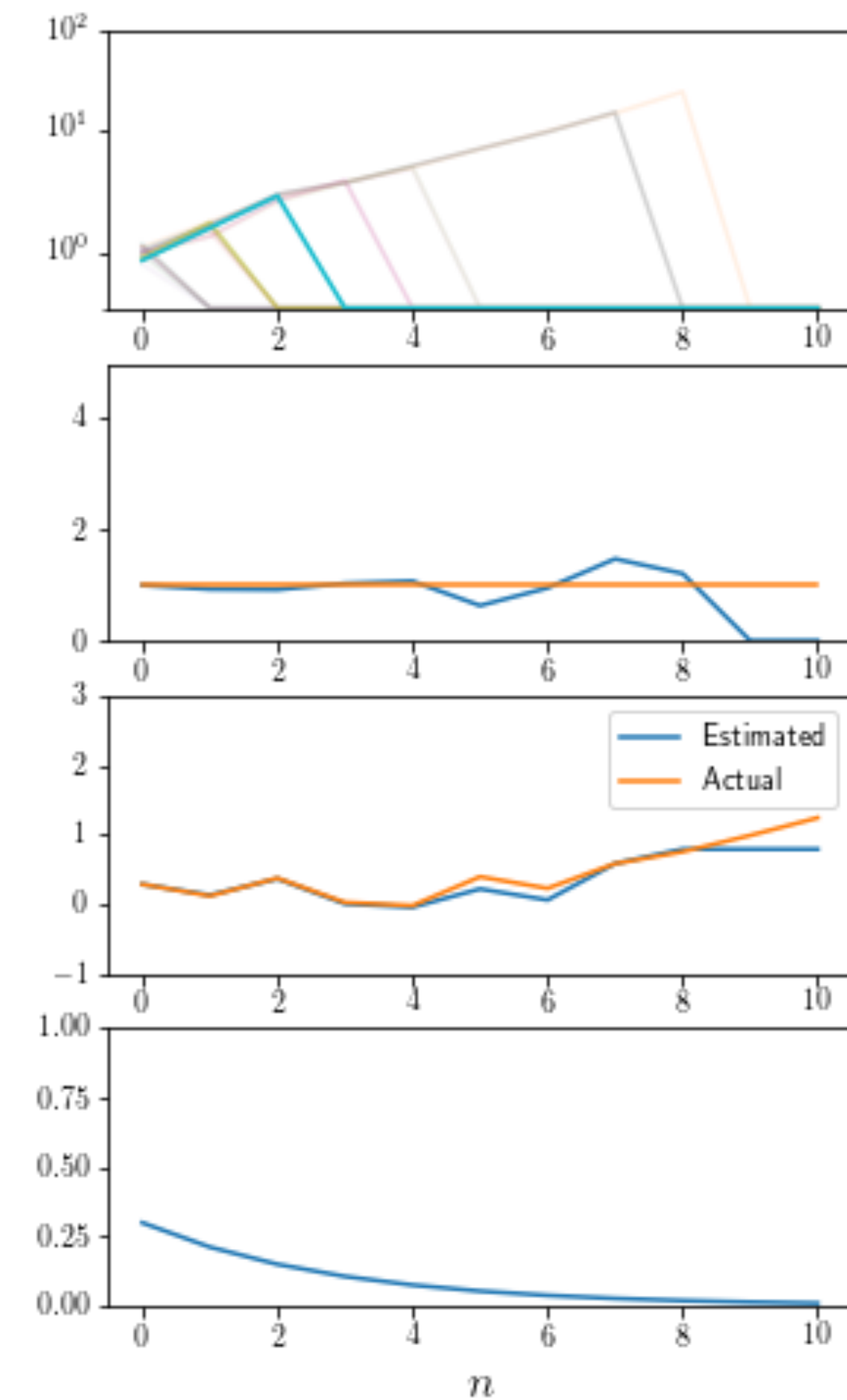
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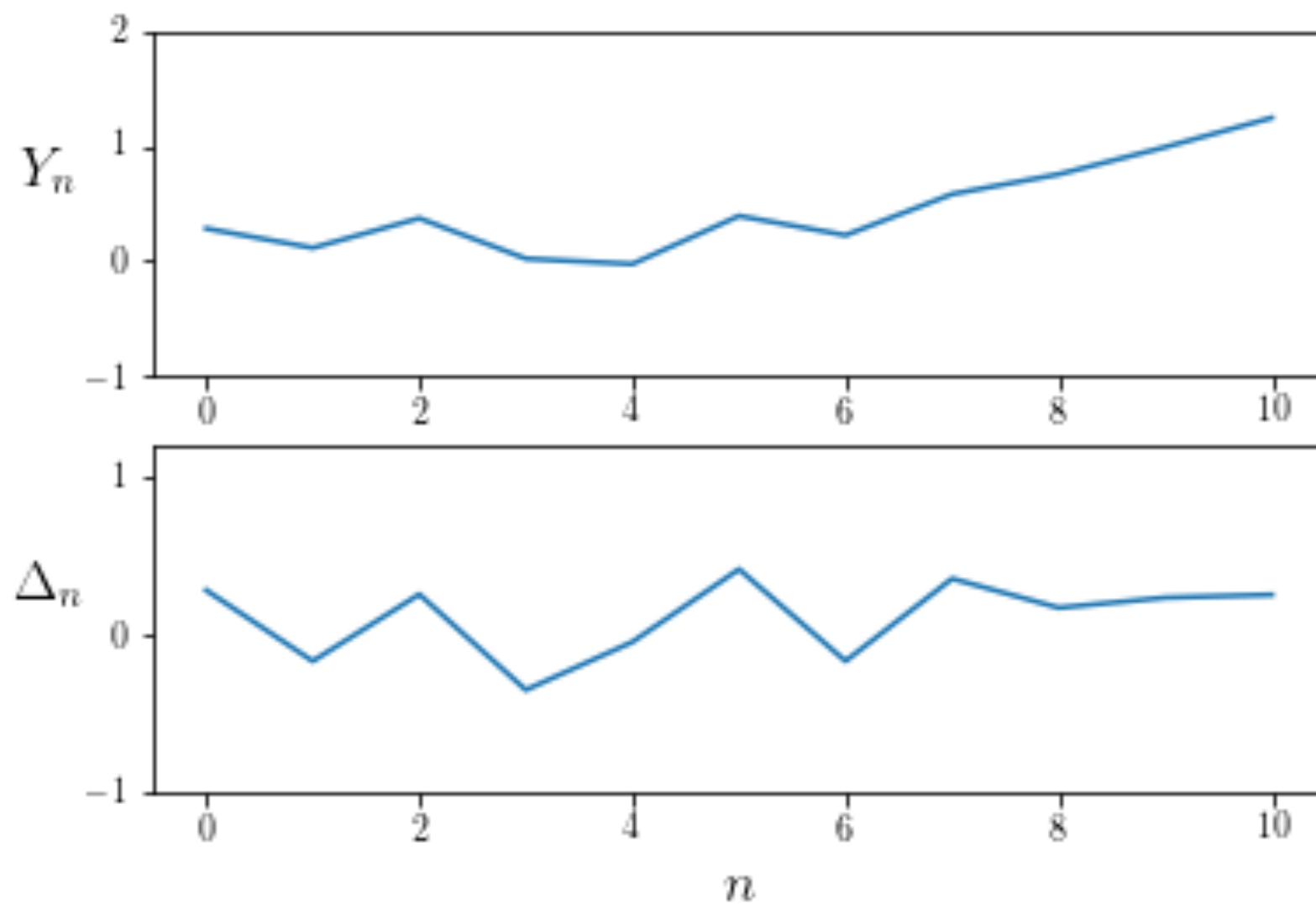
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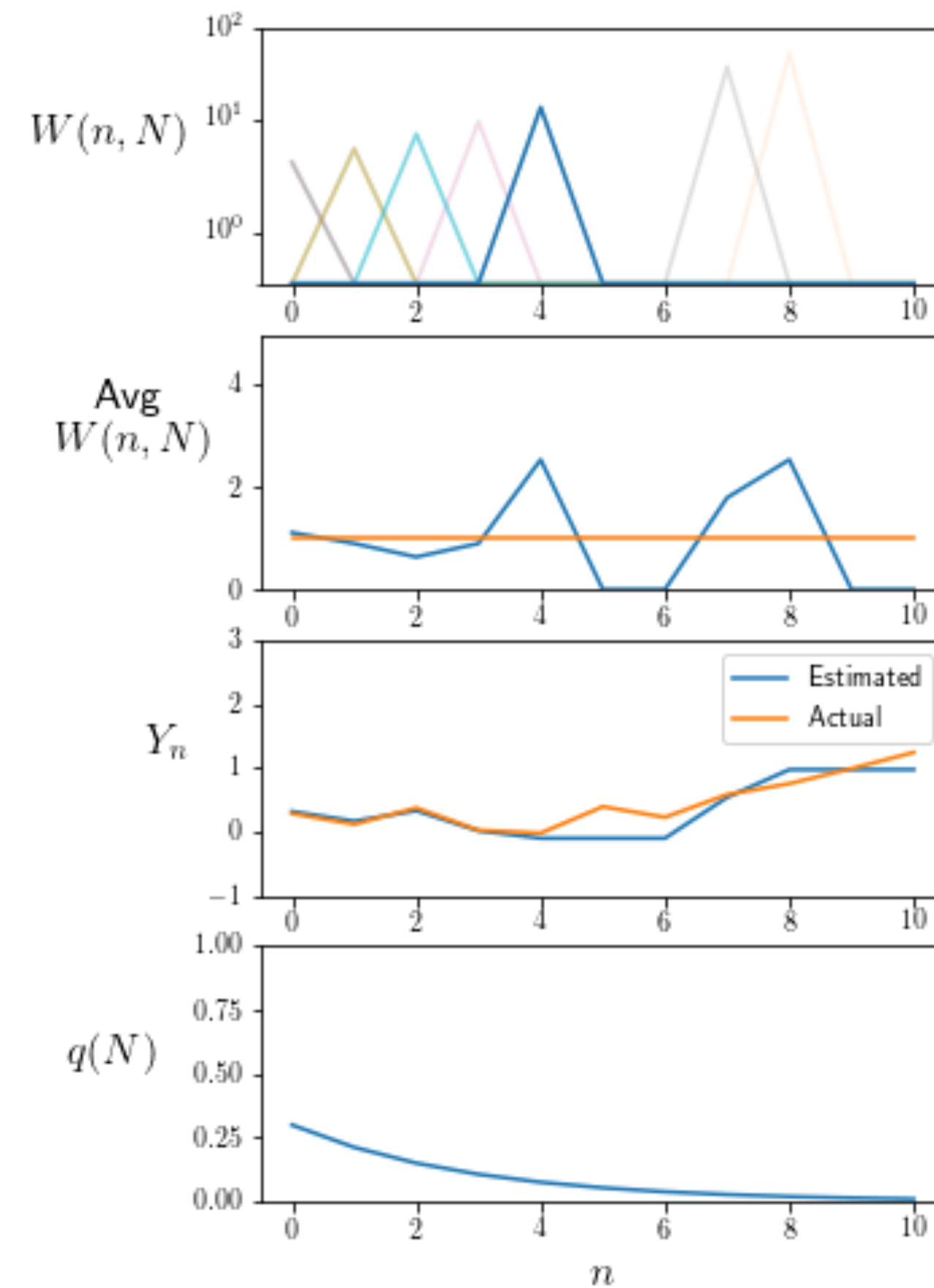
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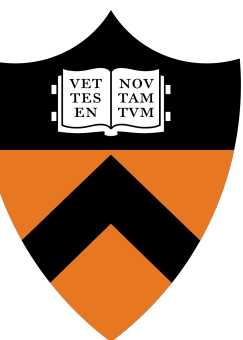
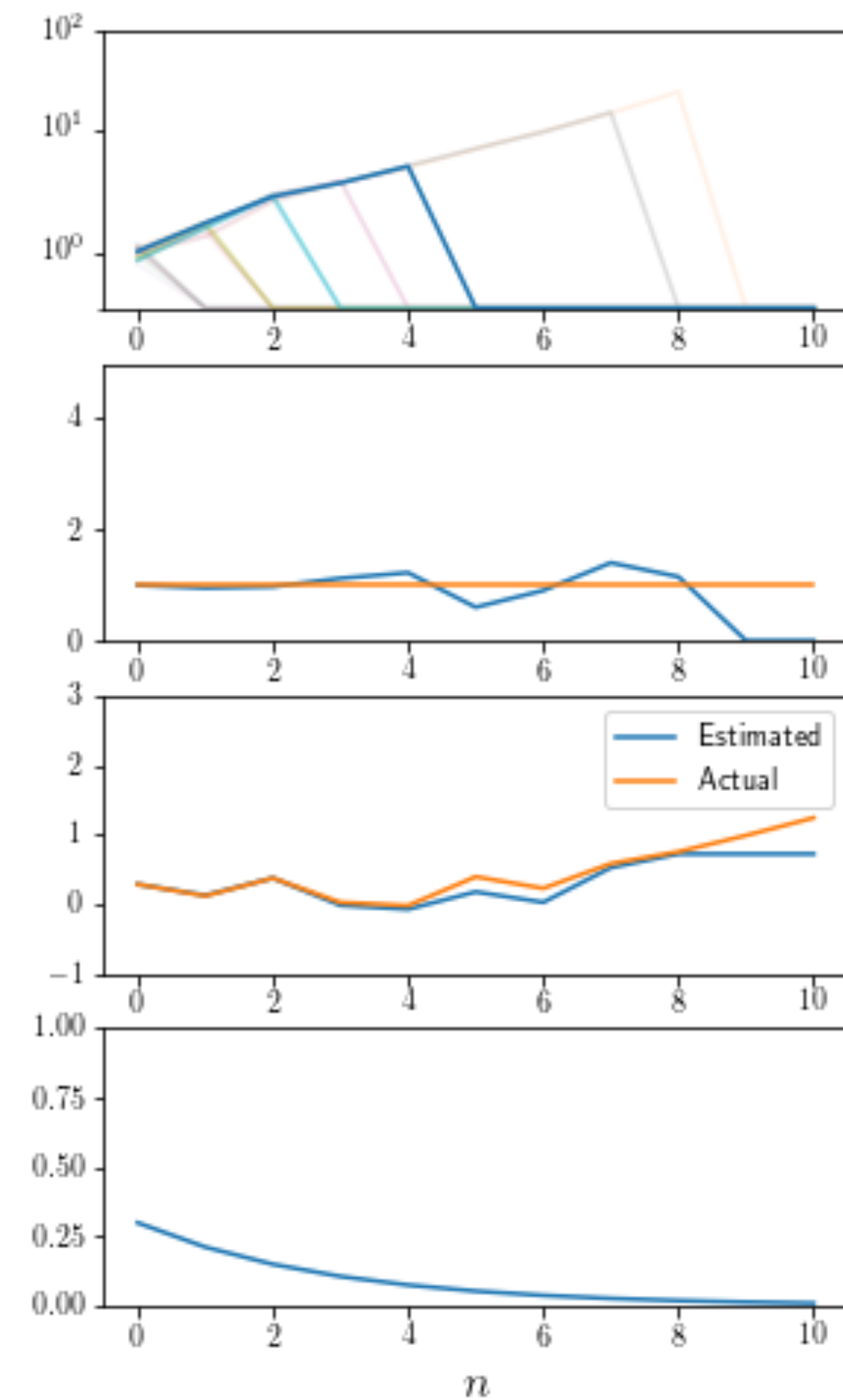
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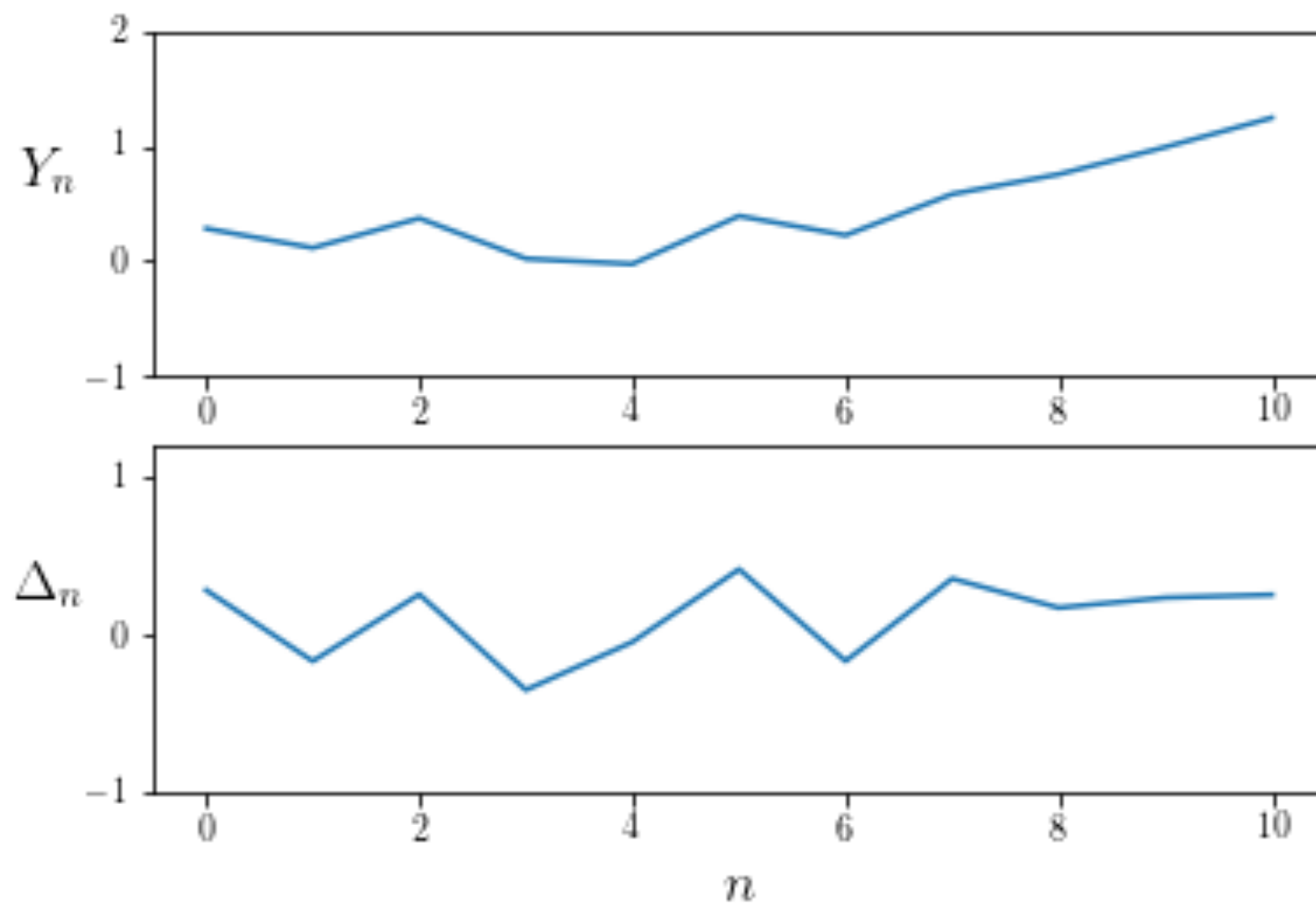
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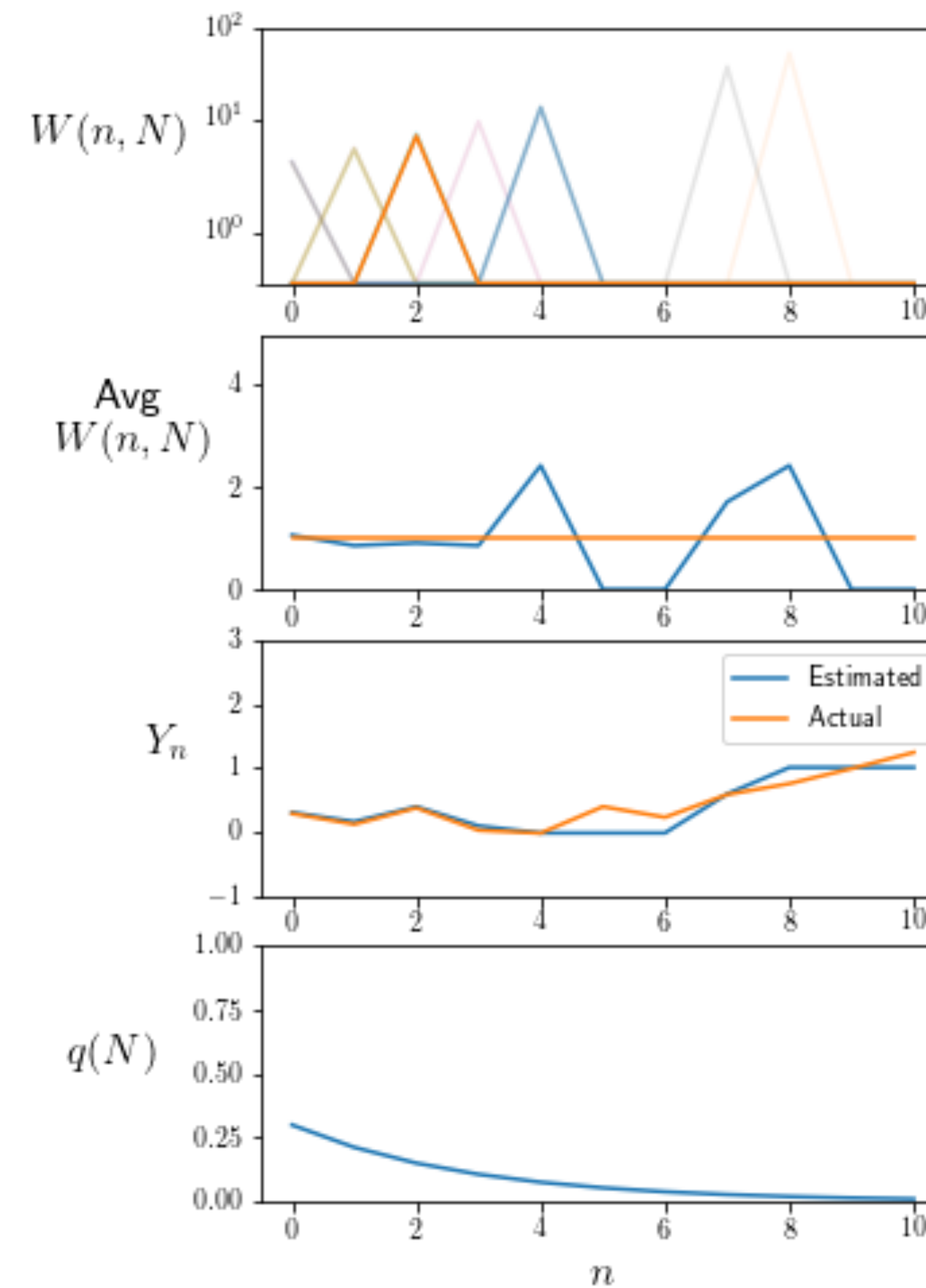
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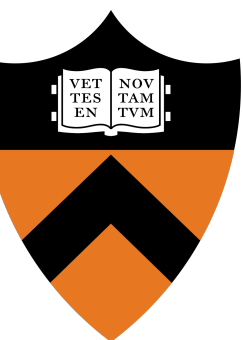
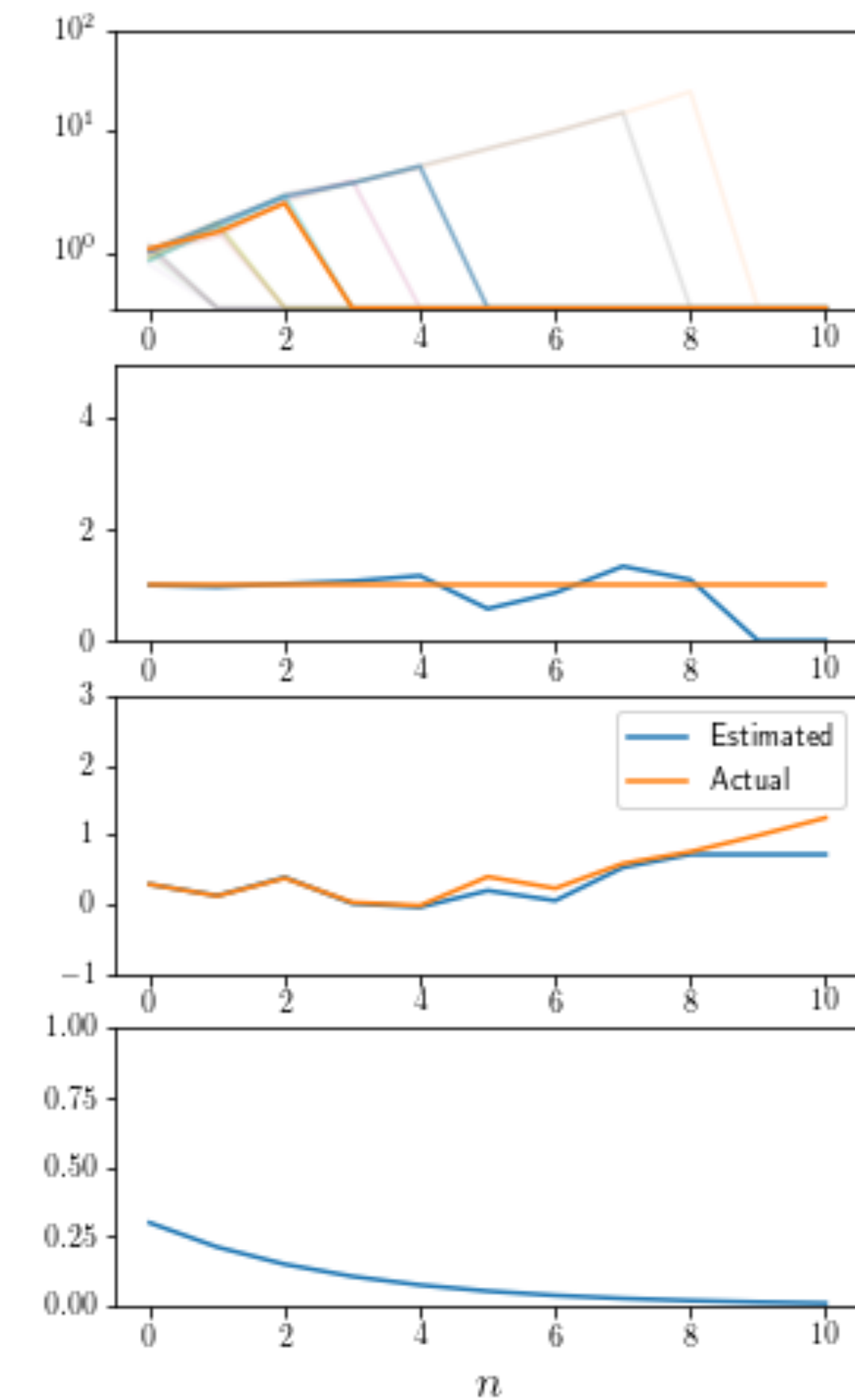
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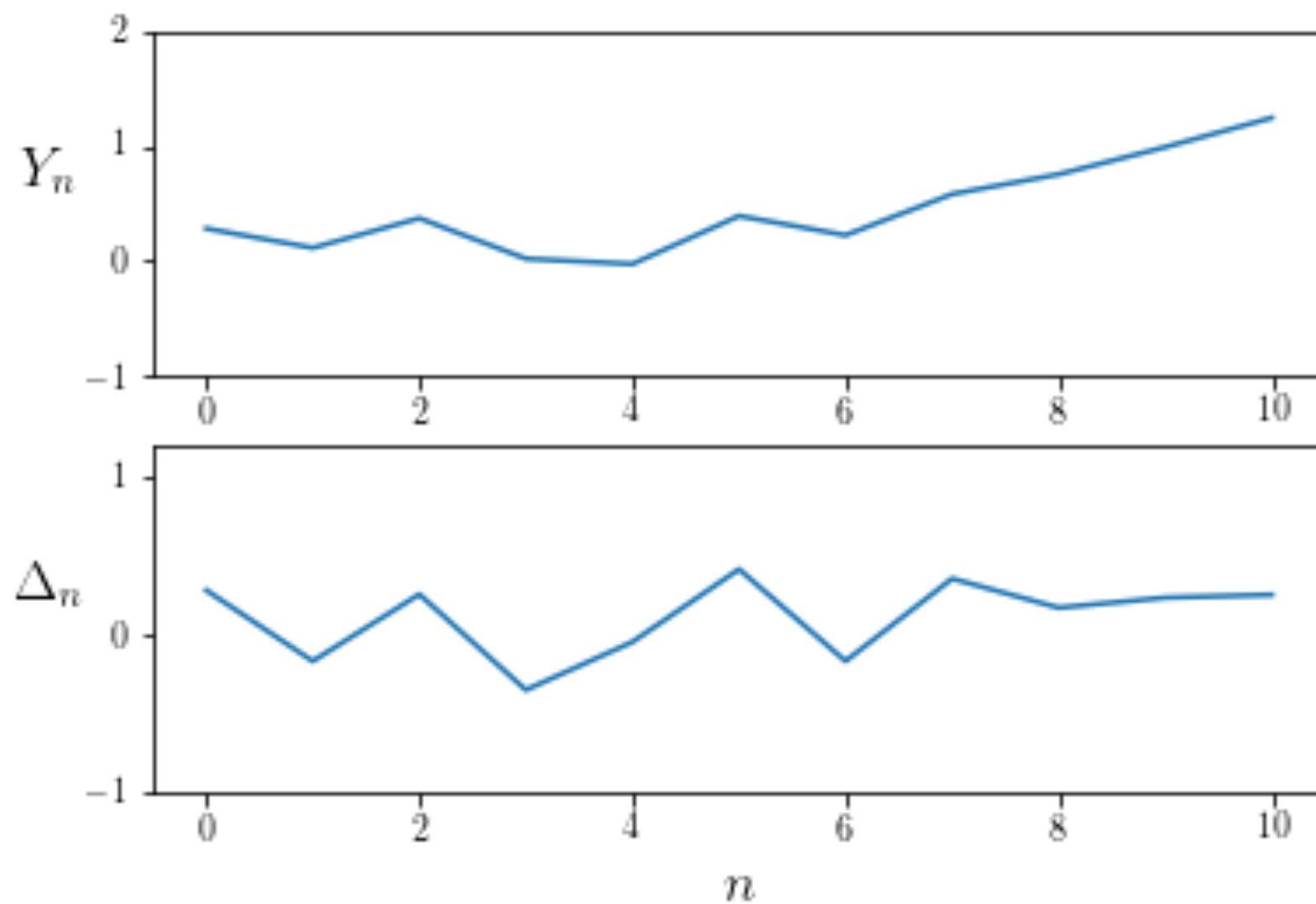
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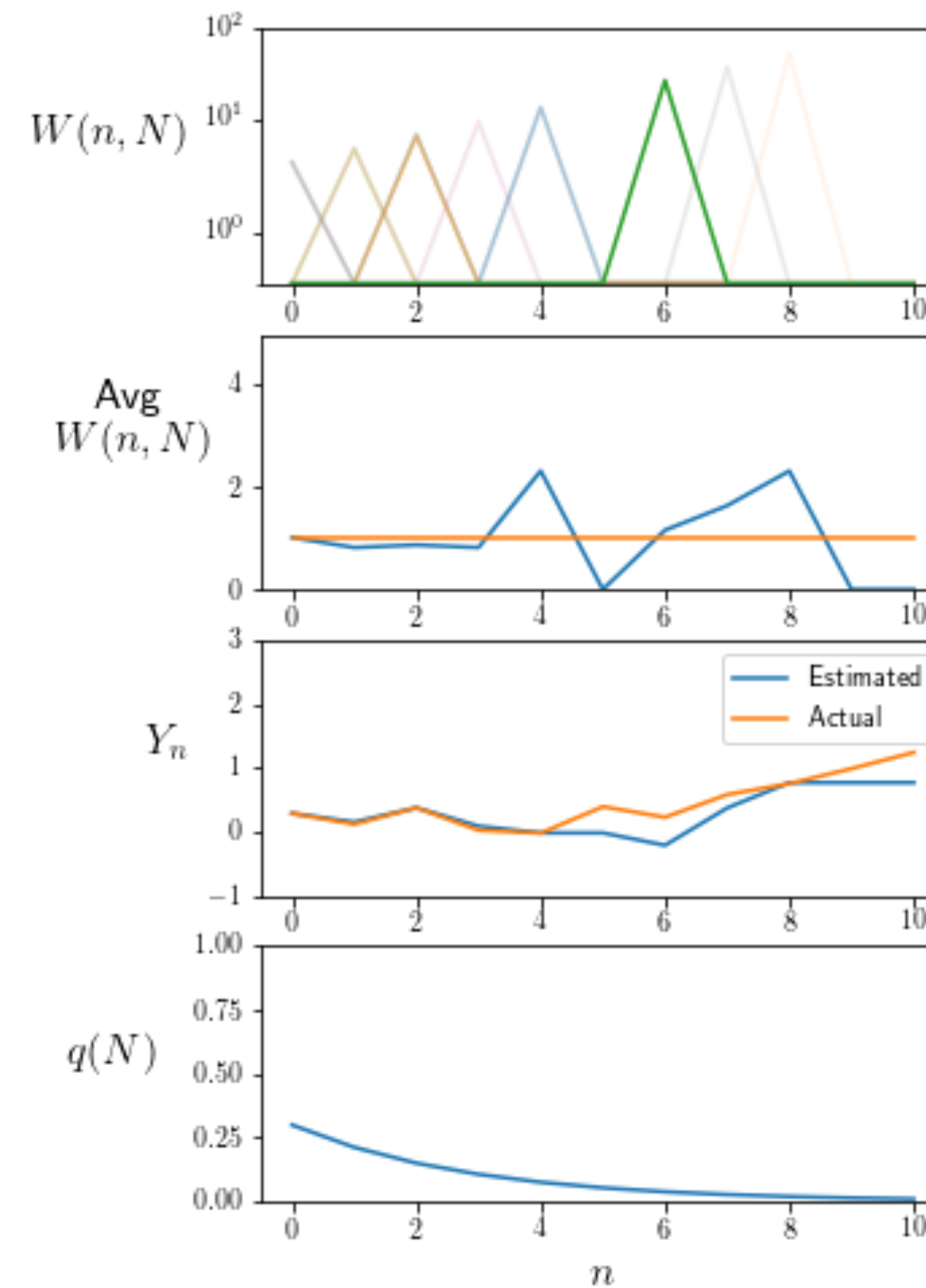
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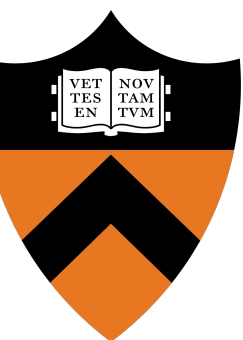
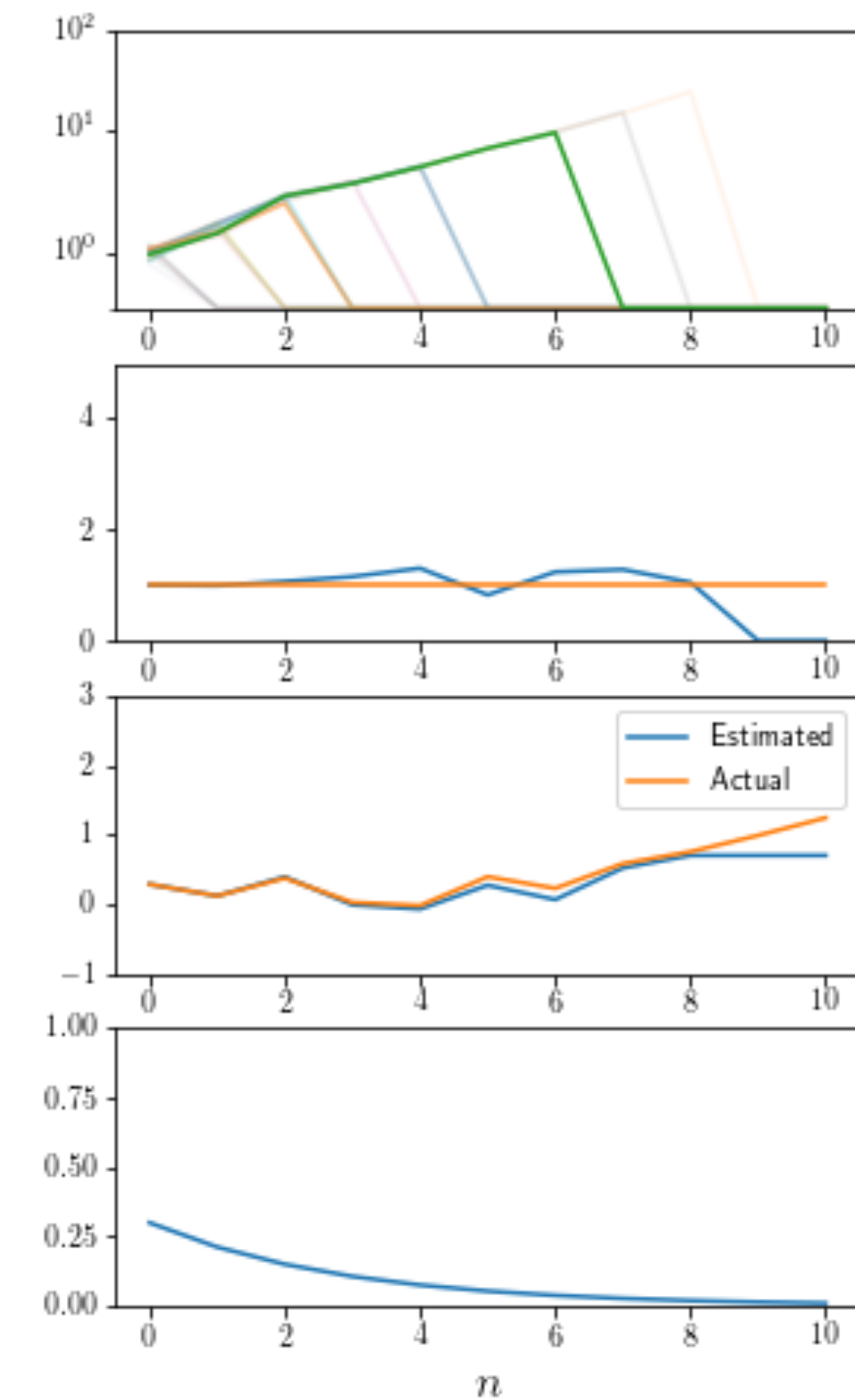
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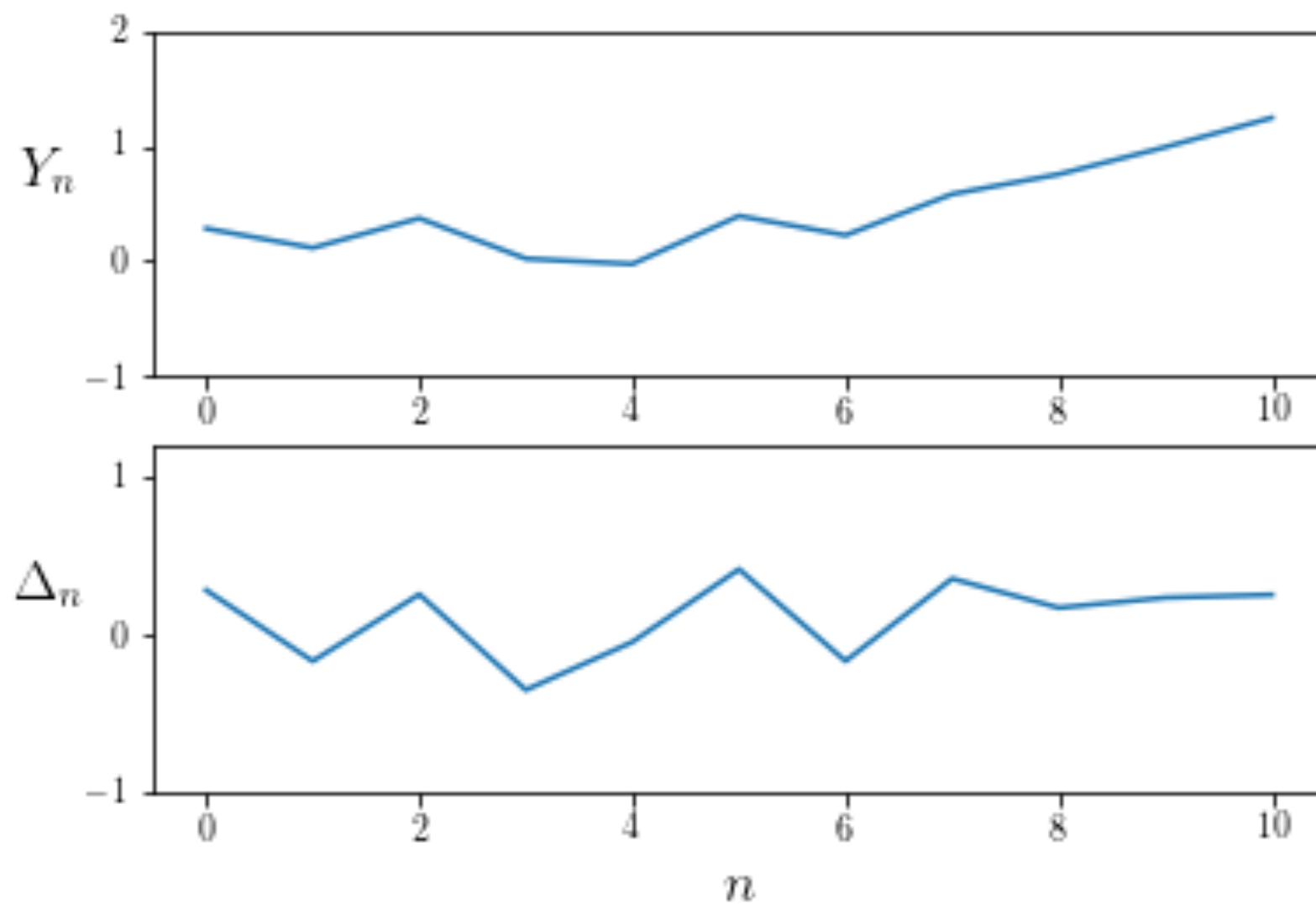
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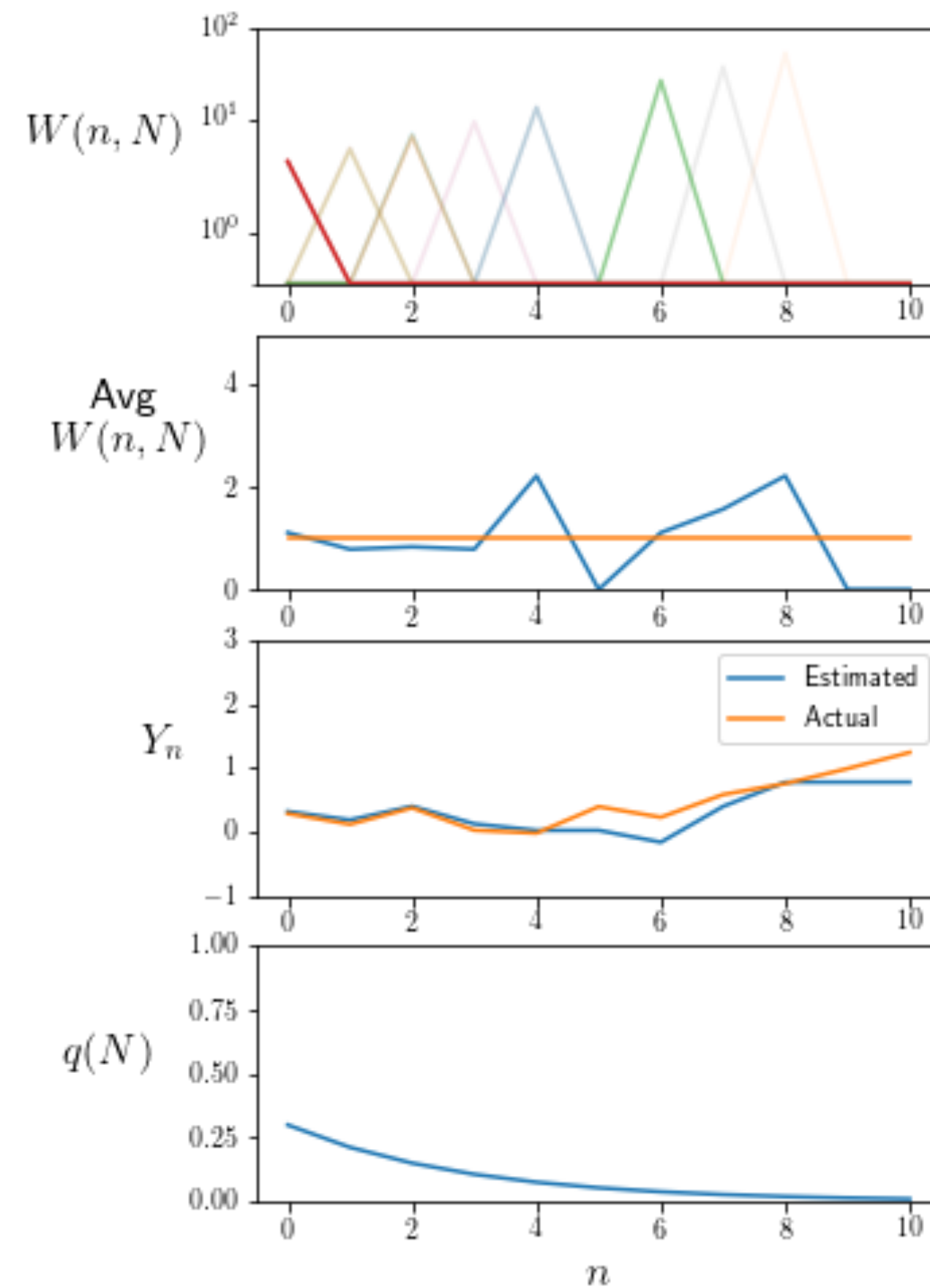
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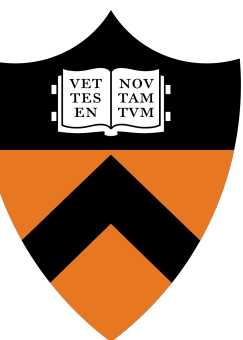
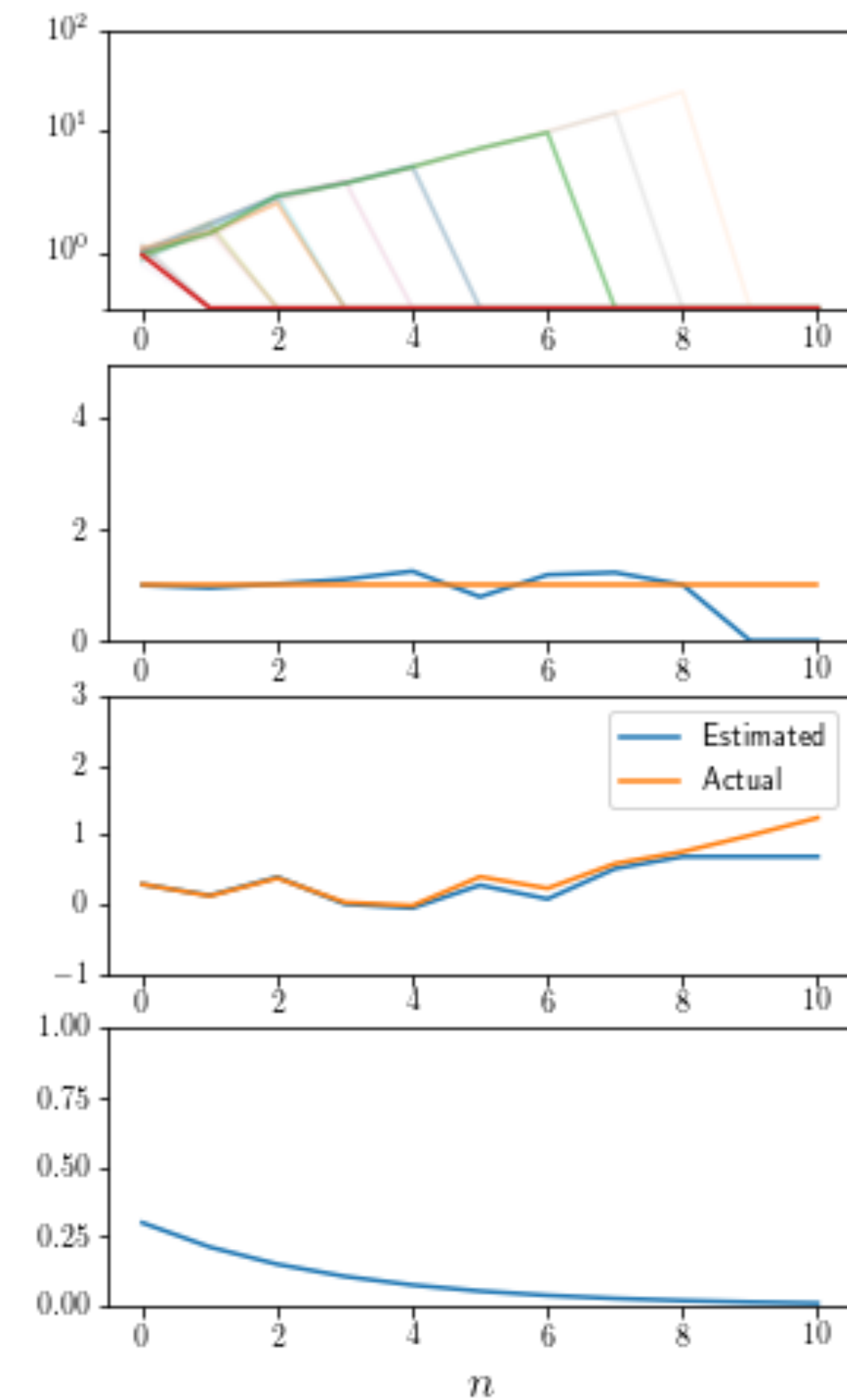
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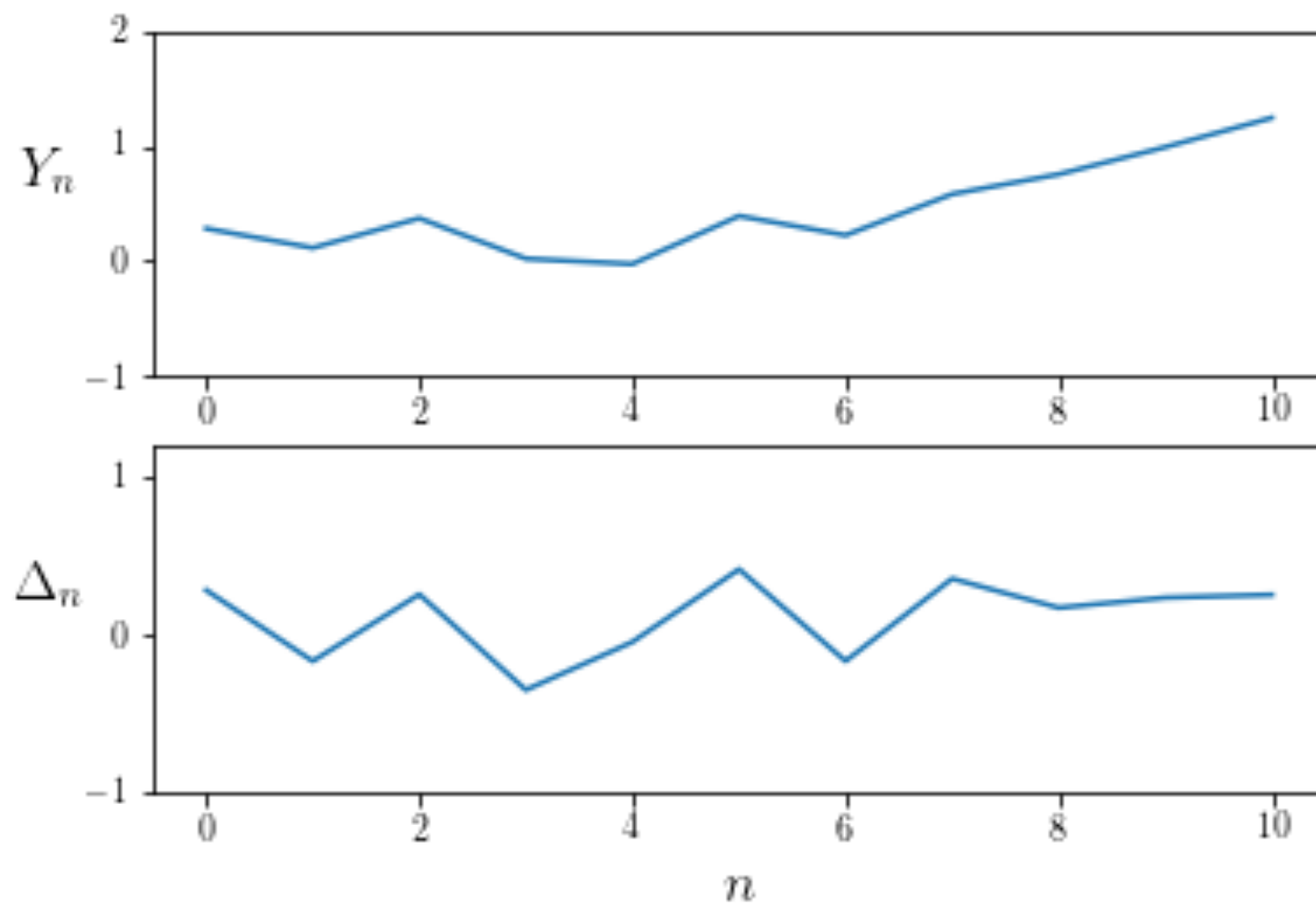
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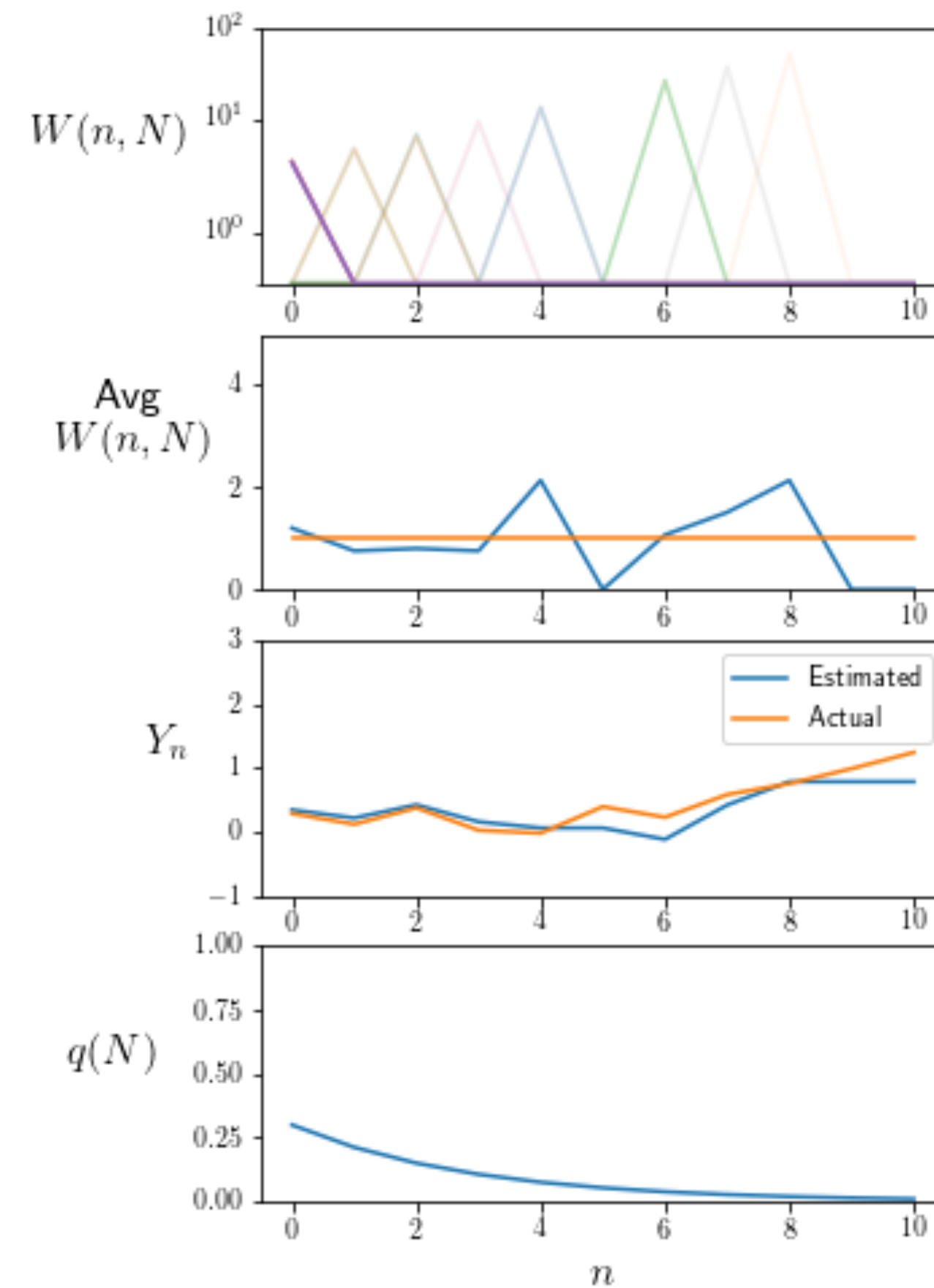
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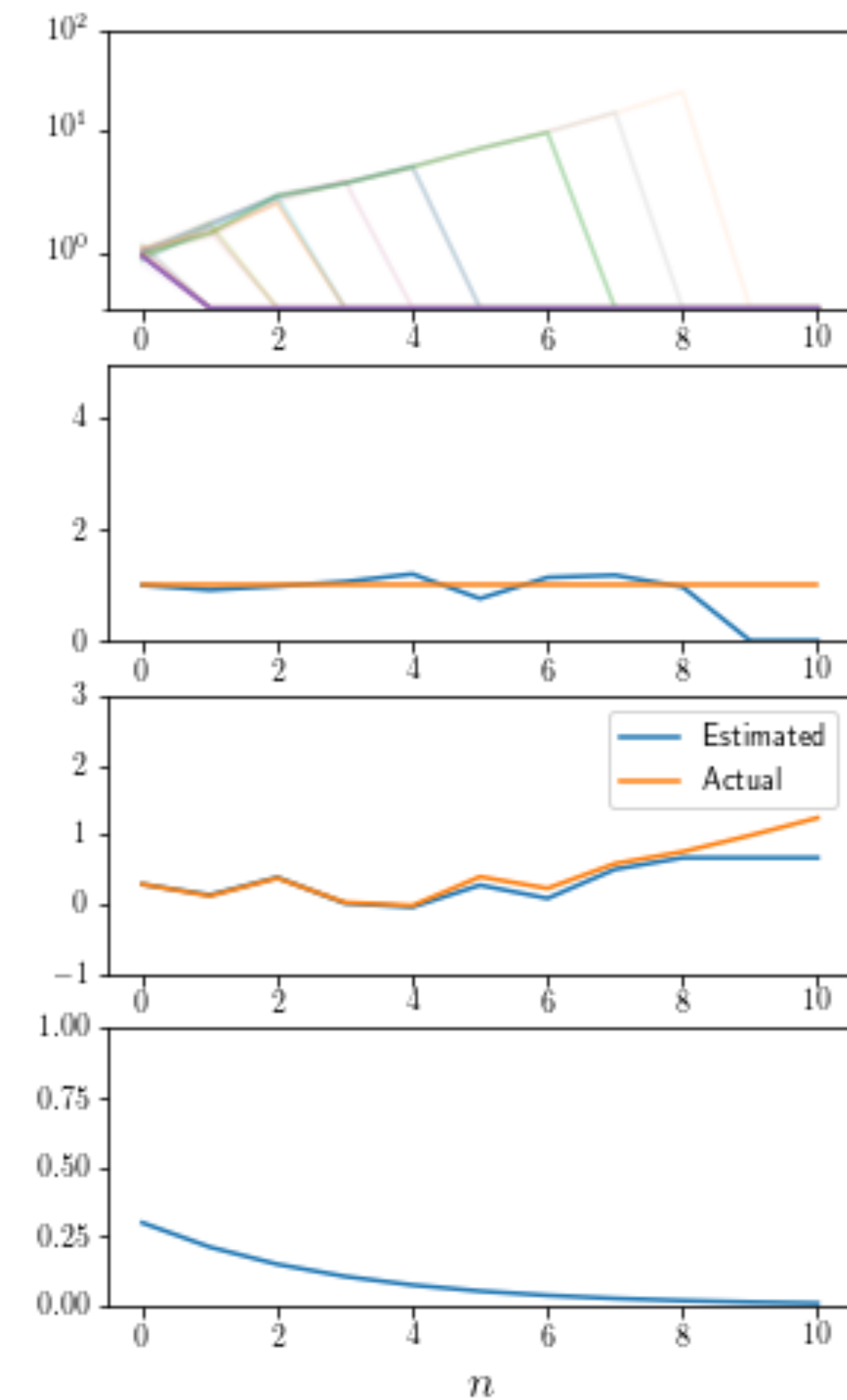
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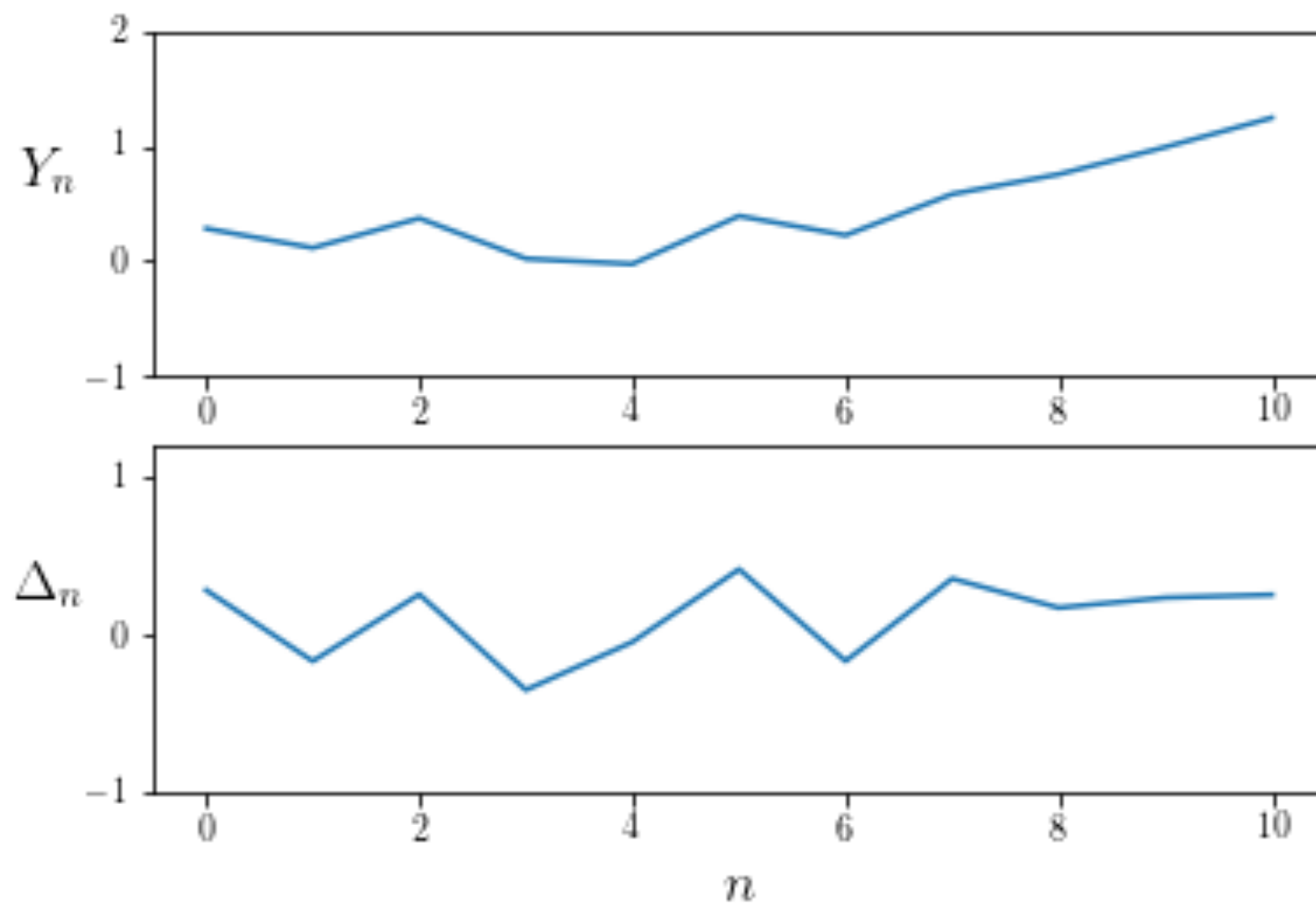
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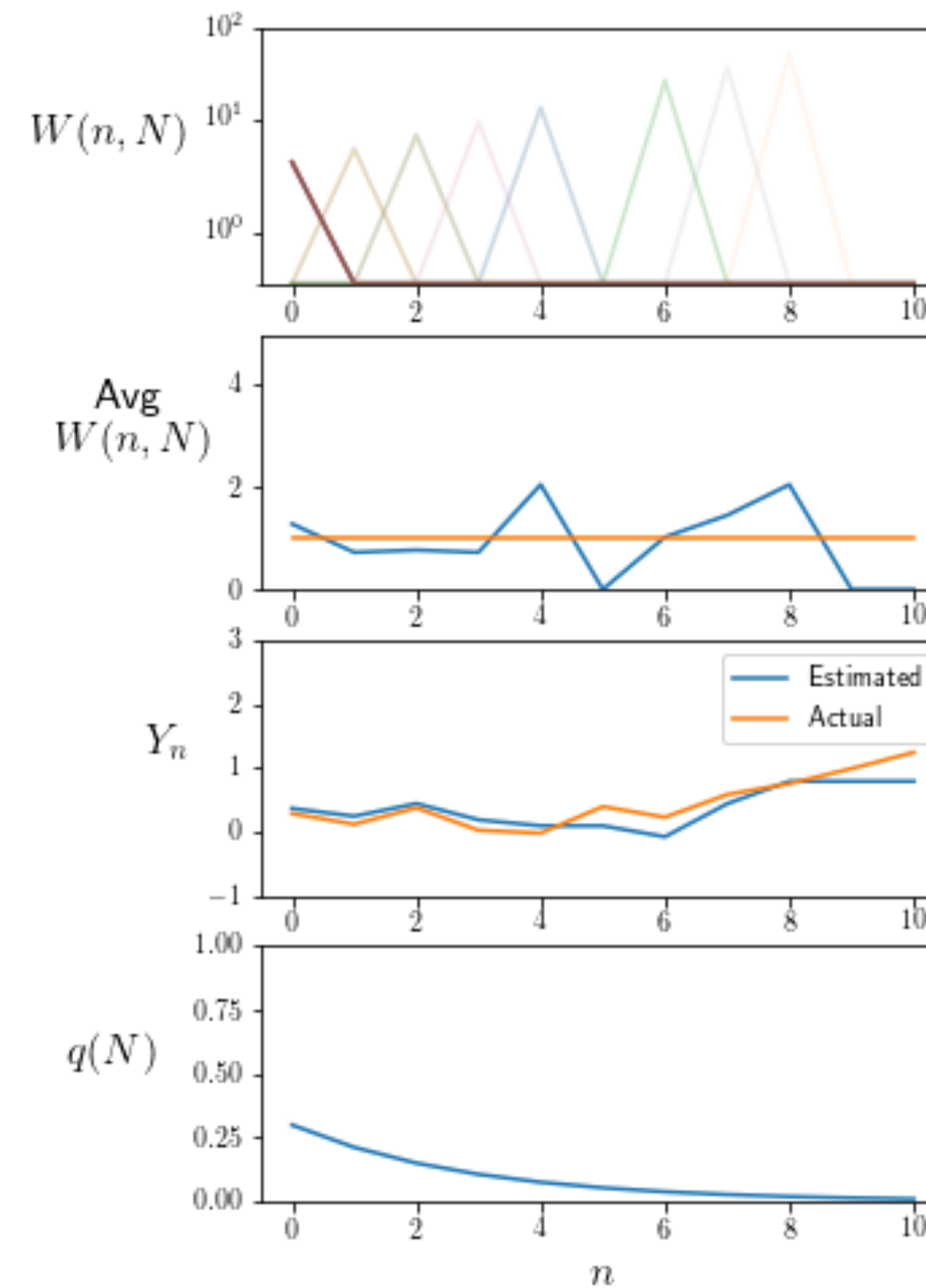
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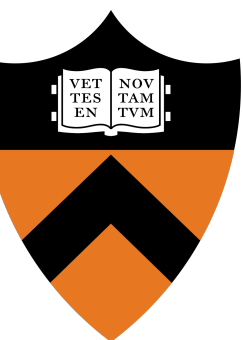
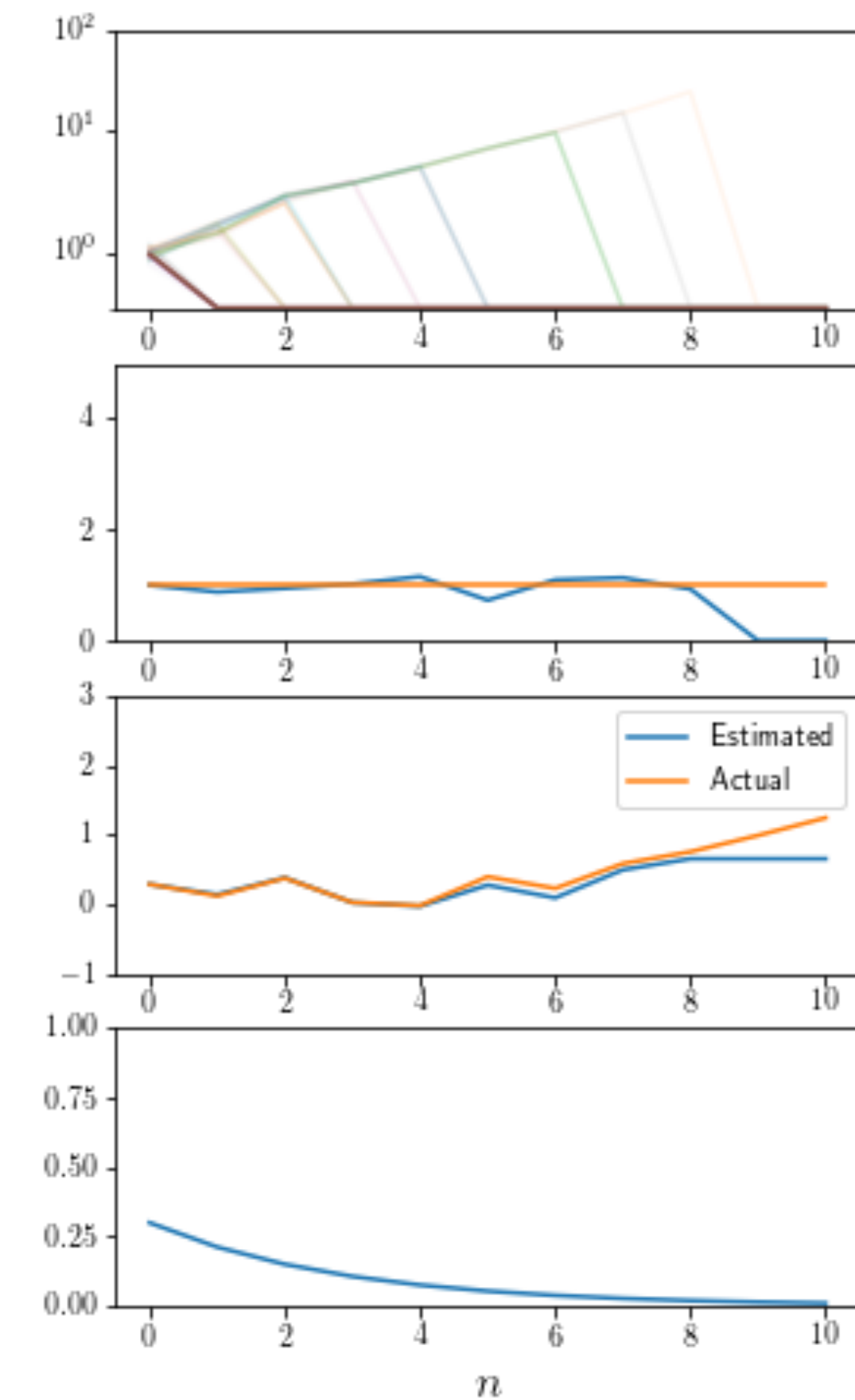
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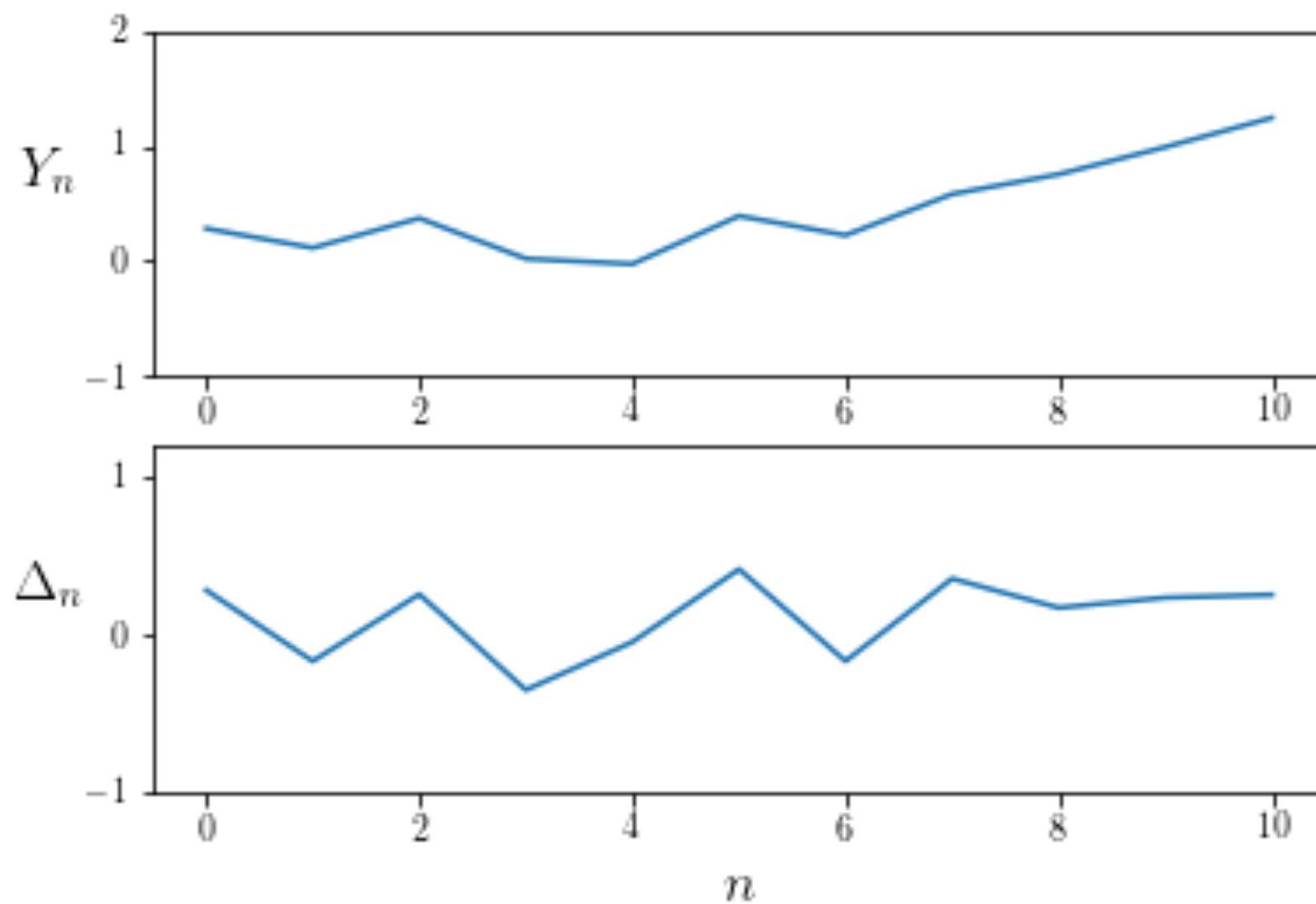
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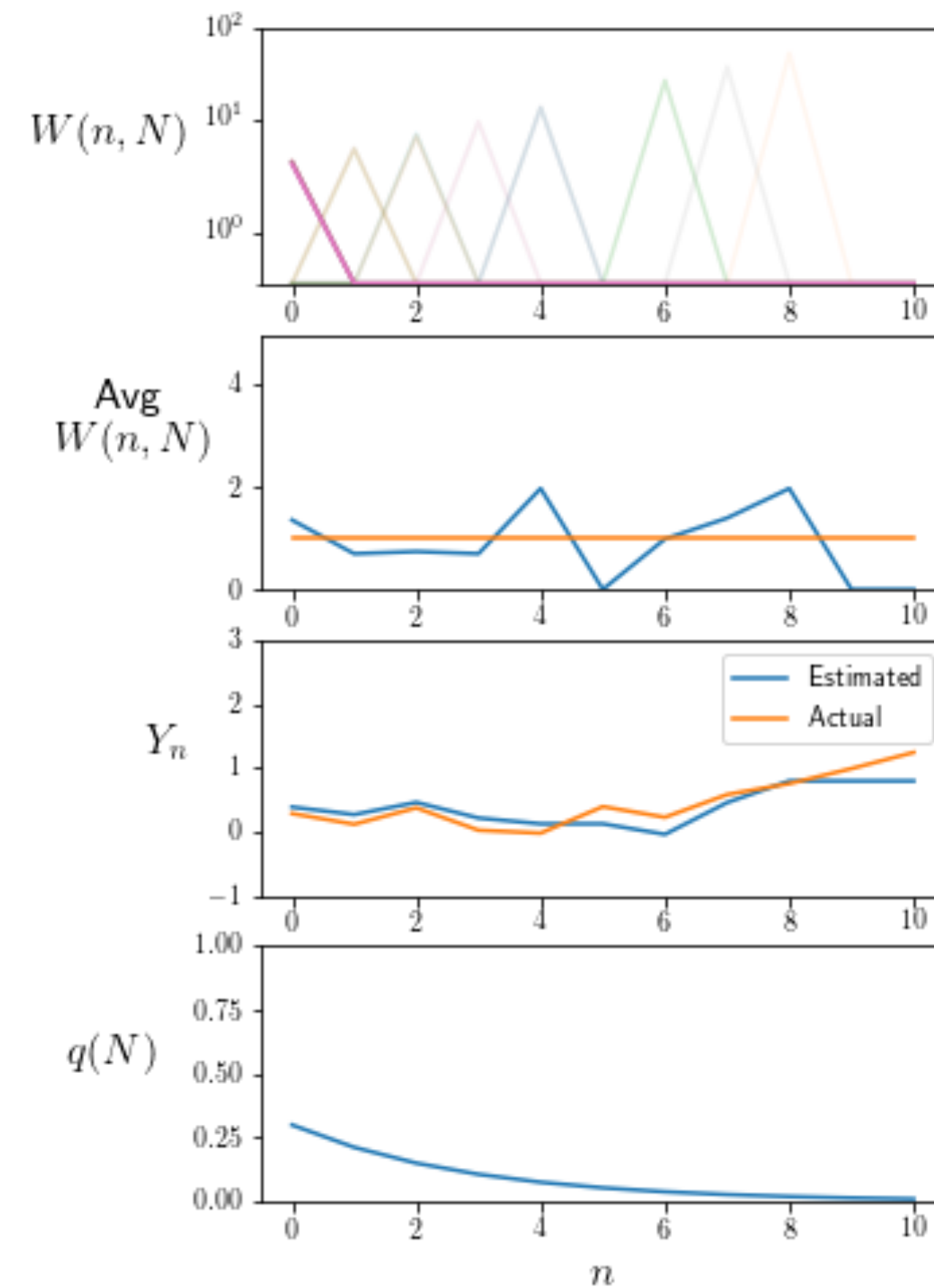
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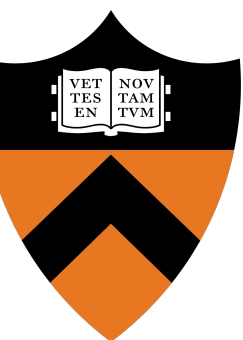
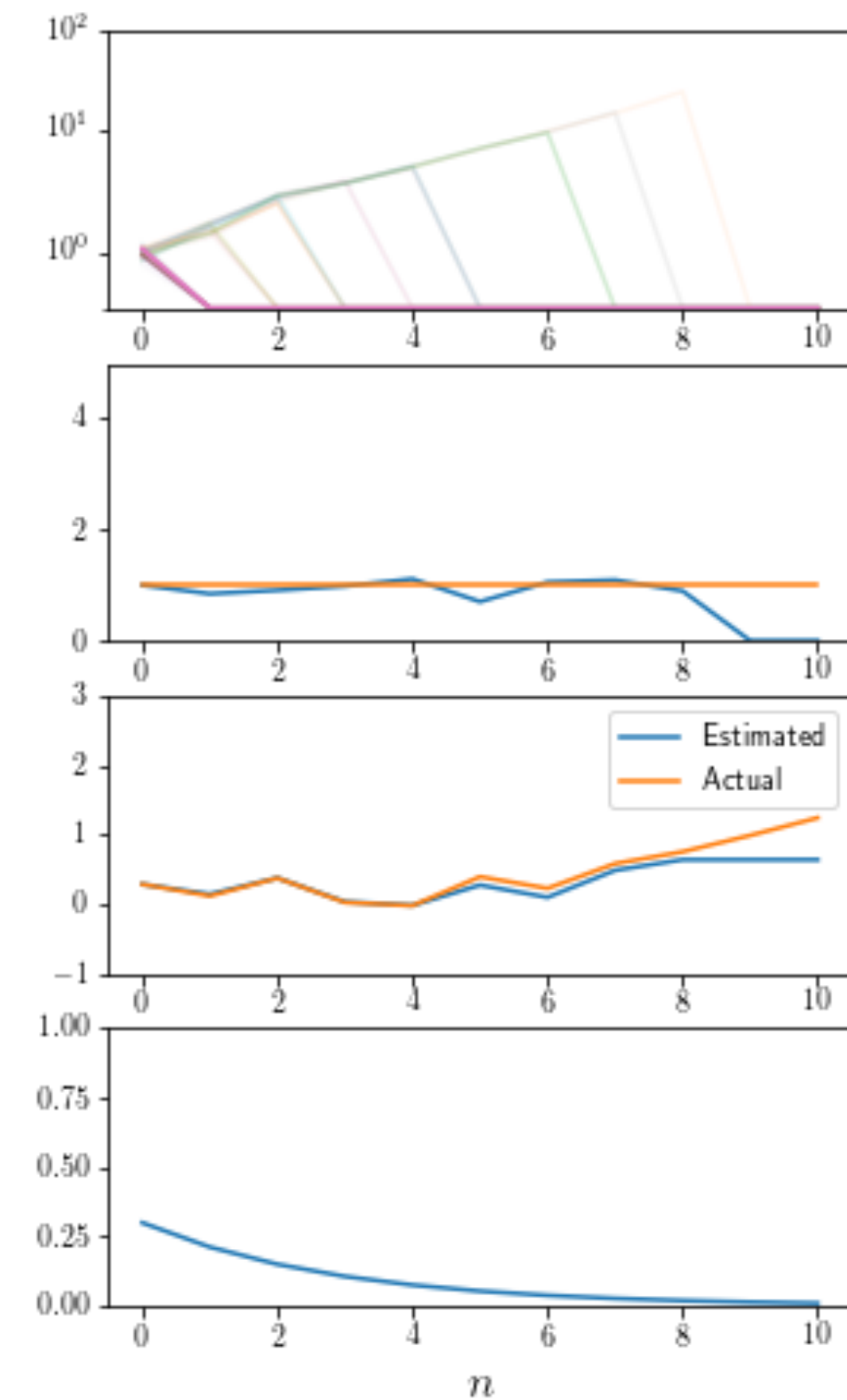
“Single sample”

$$W(n, N) = \frac{1}{q(N)} \mathbb{1}\{n = N\}$$



“Russian roulette”

$$W(n, N) = \frac{1}{1 - \sum_{n'=1}^{n-1} q(n')} \mathbb{1}\{N \geq n\}$$



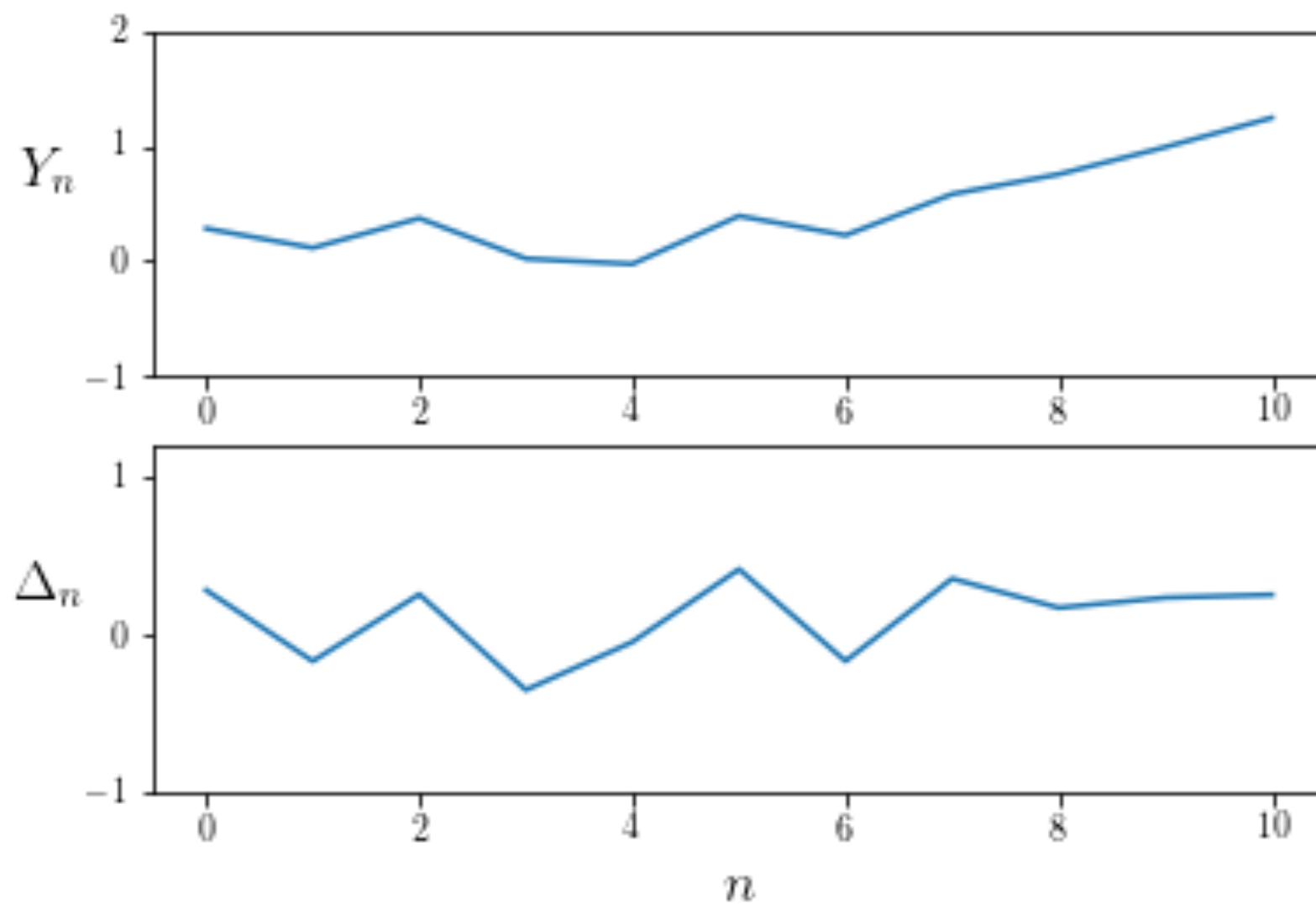
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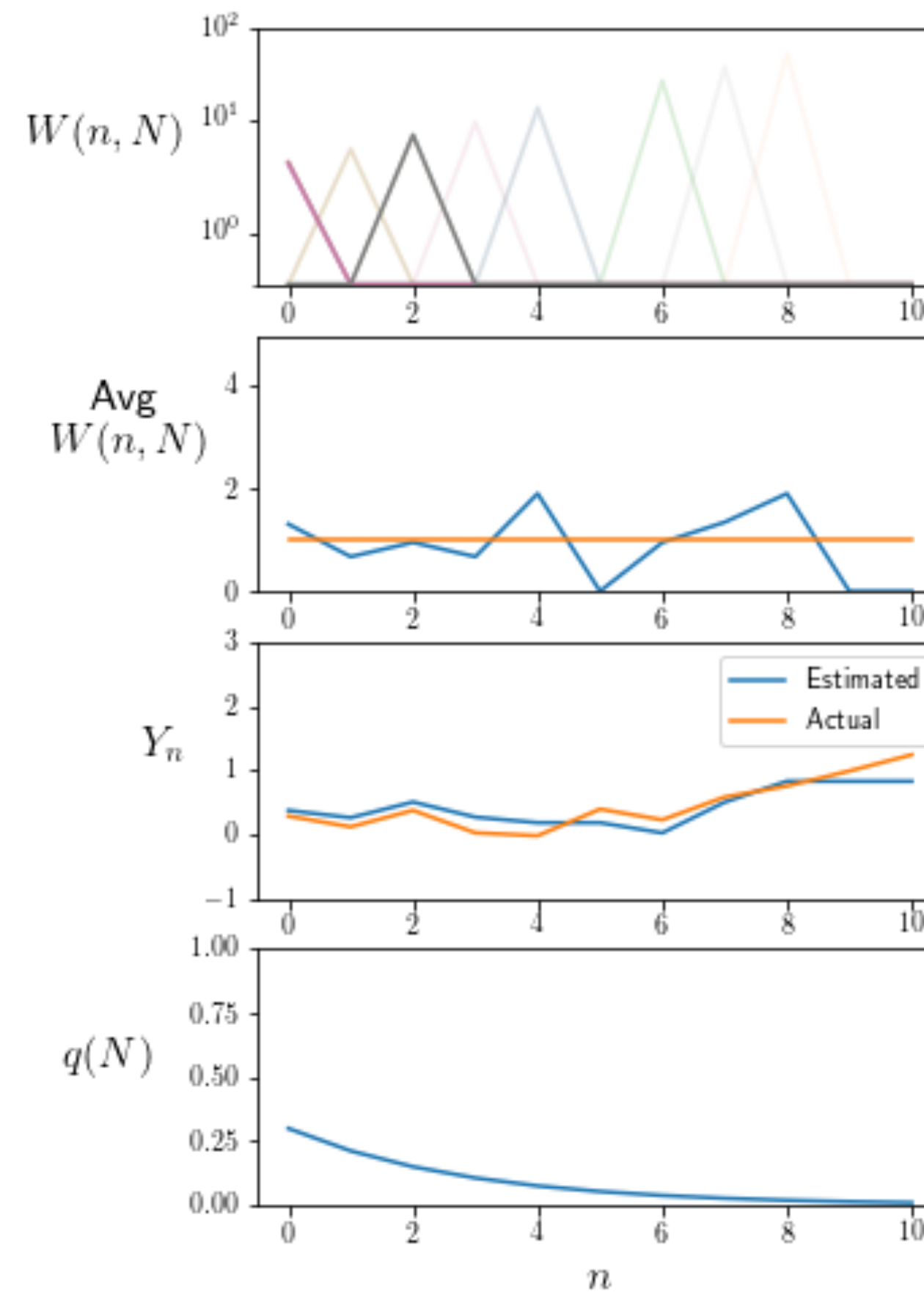
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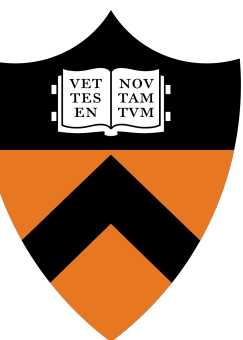
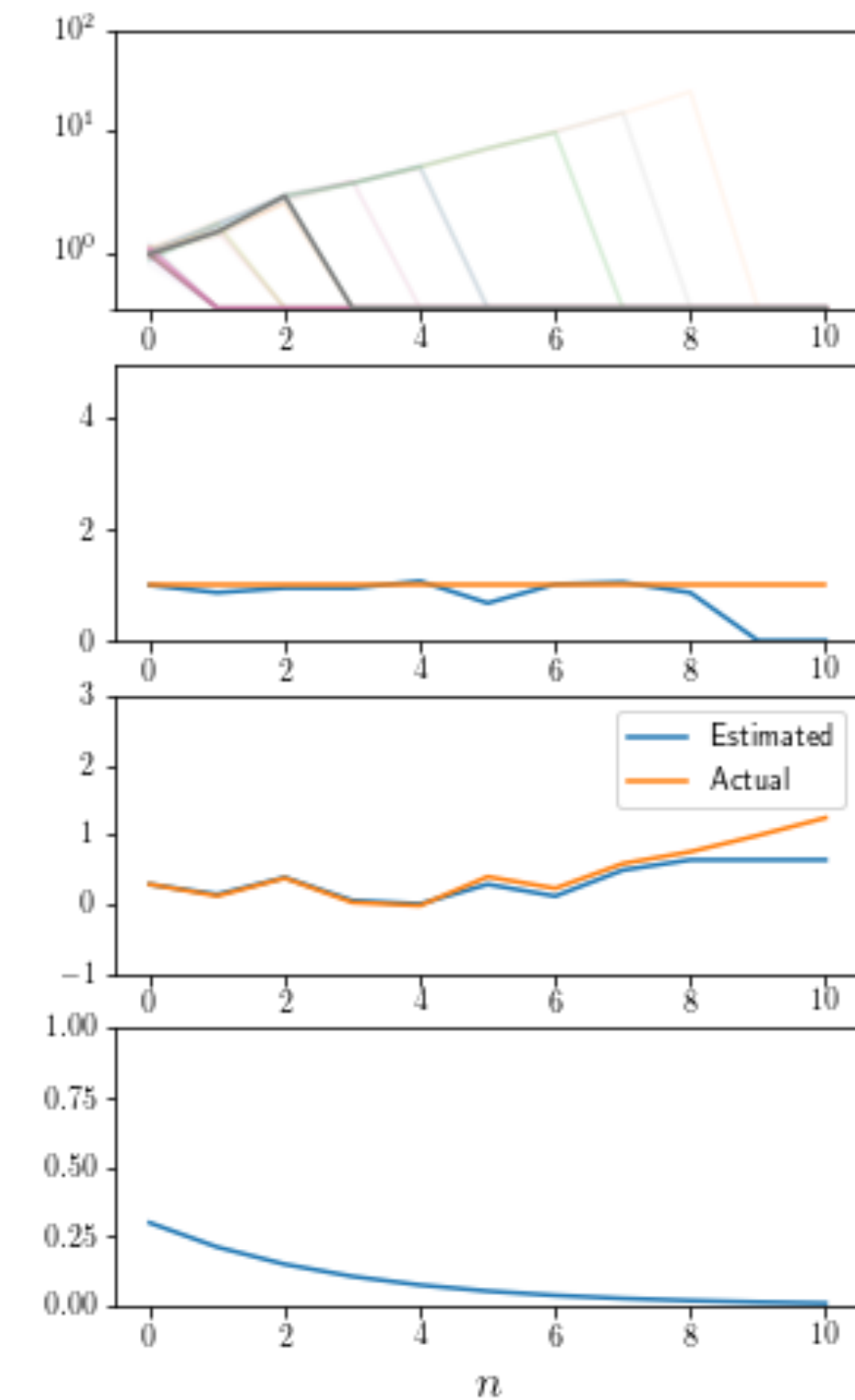
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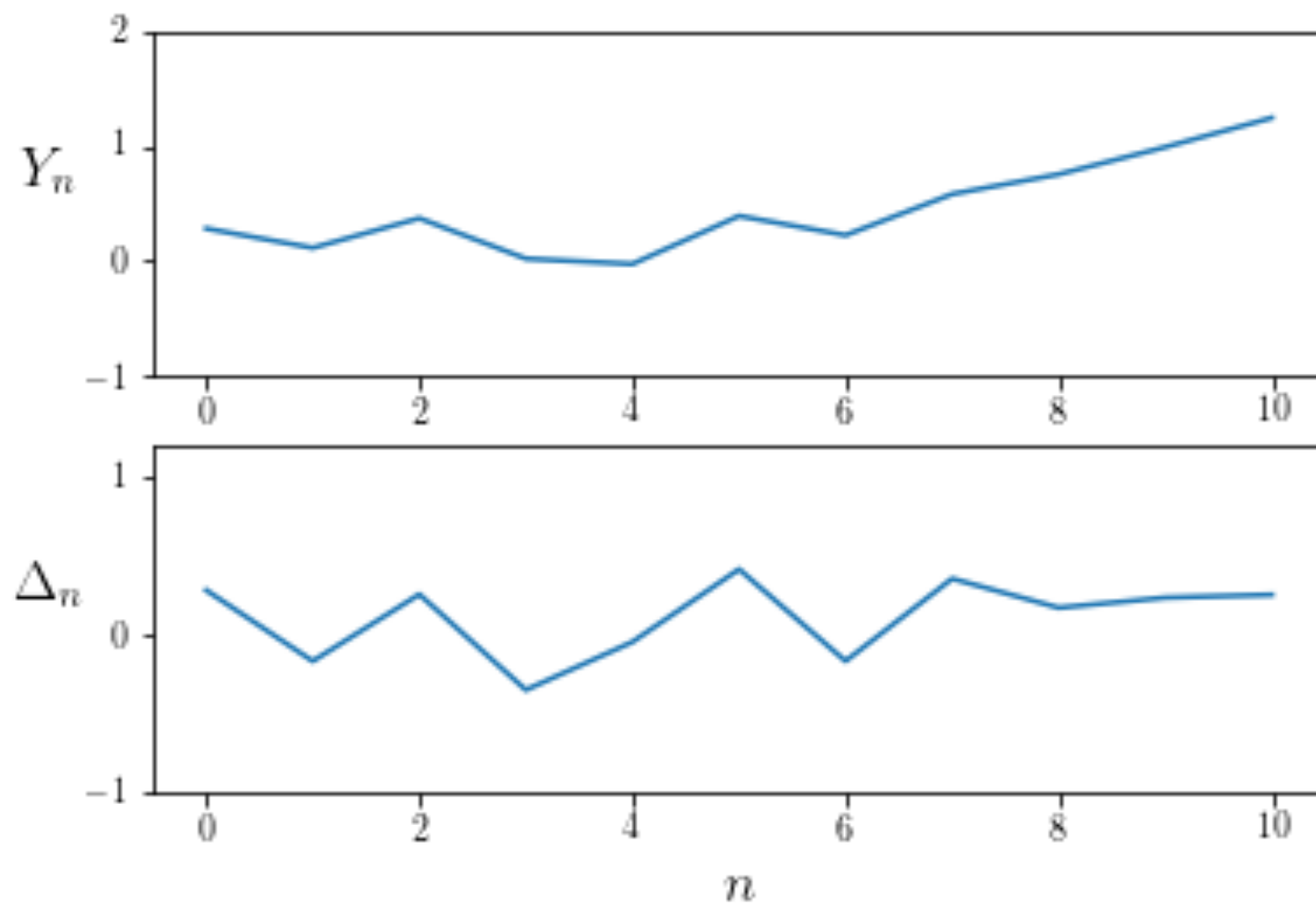
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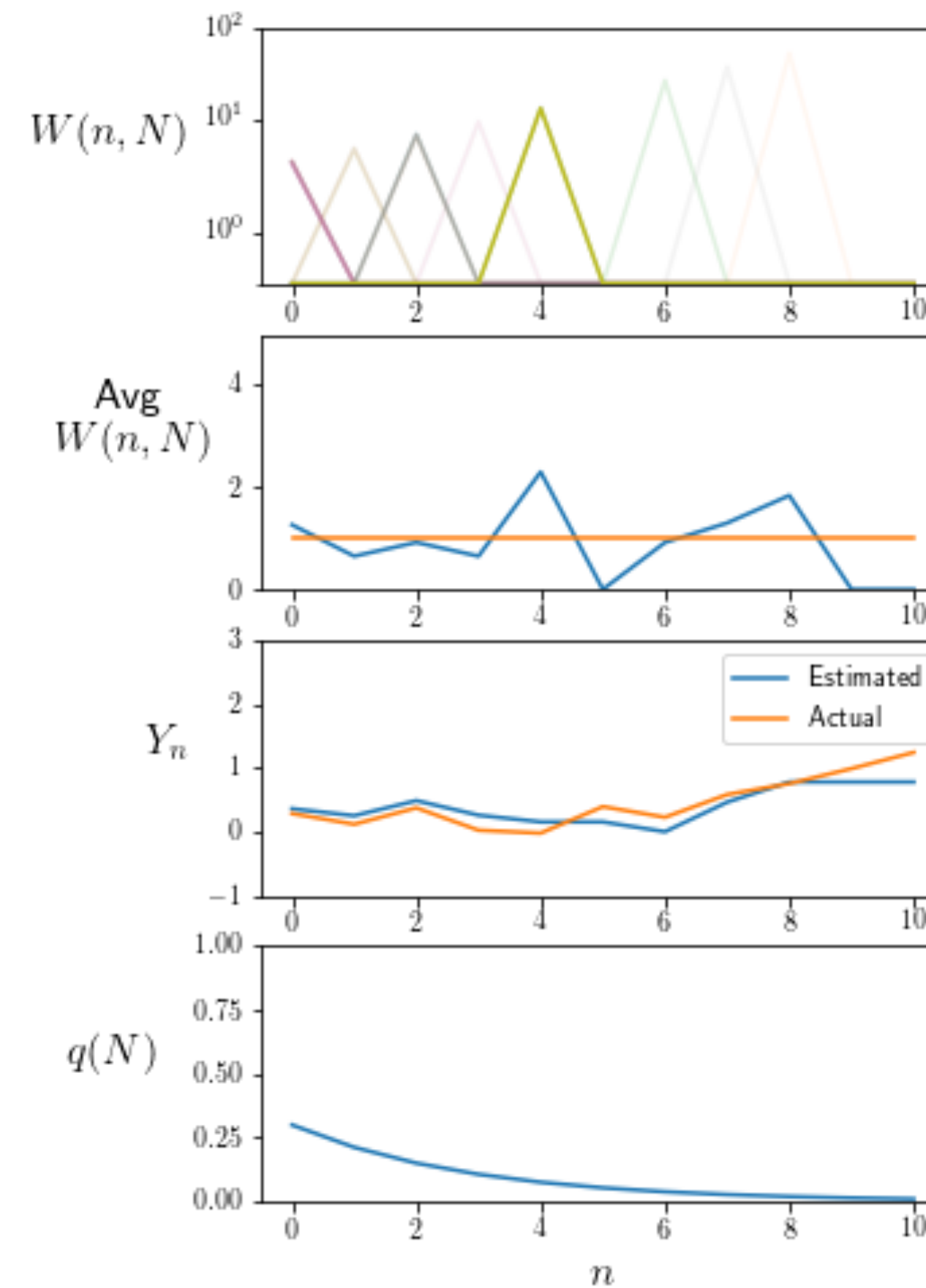
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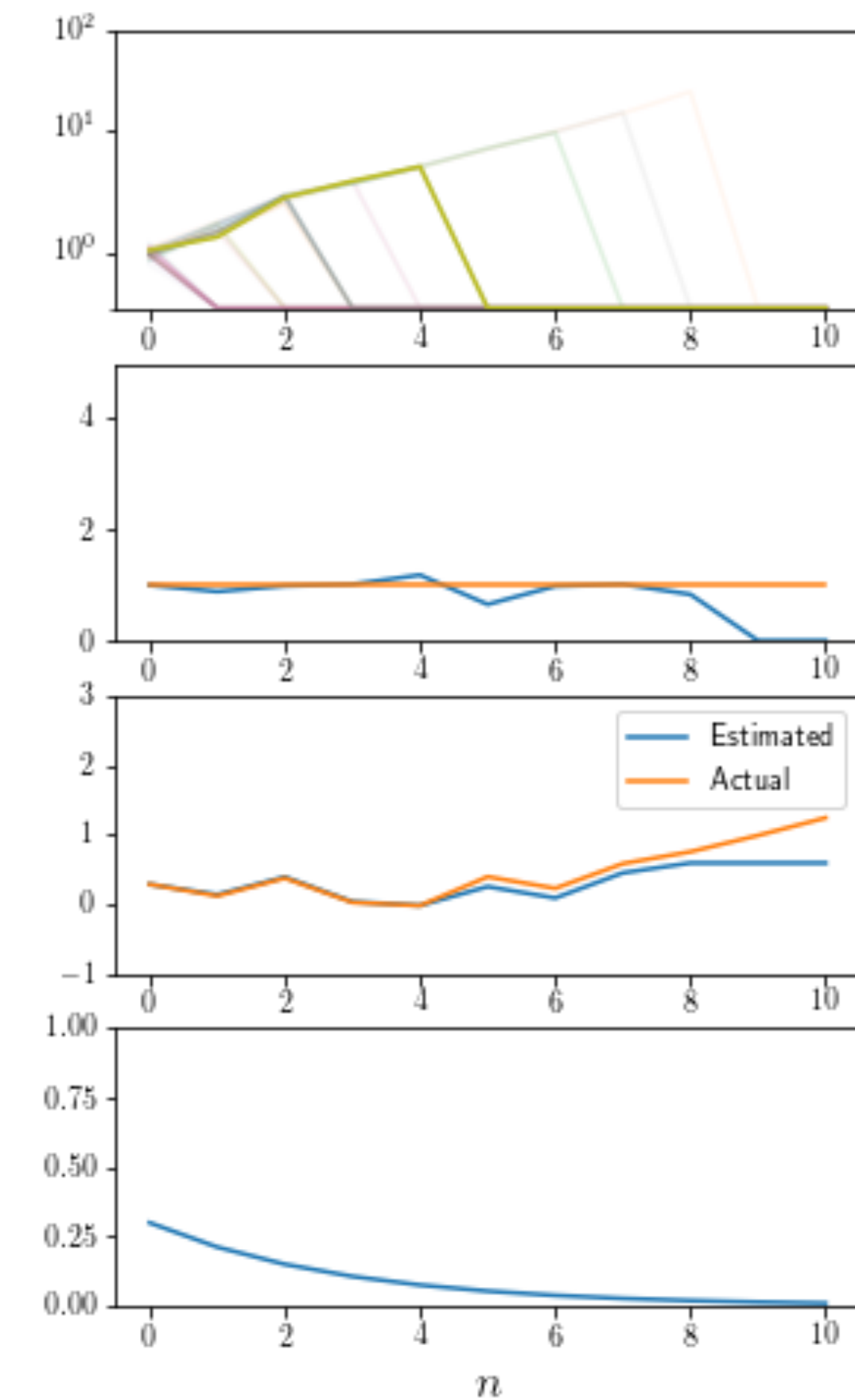
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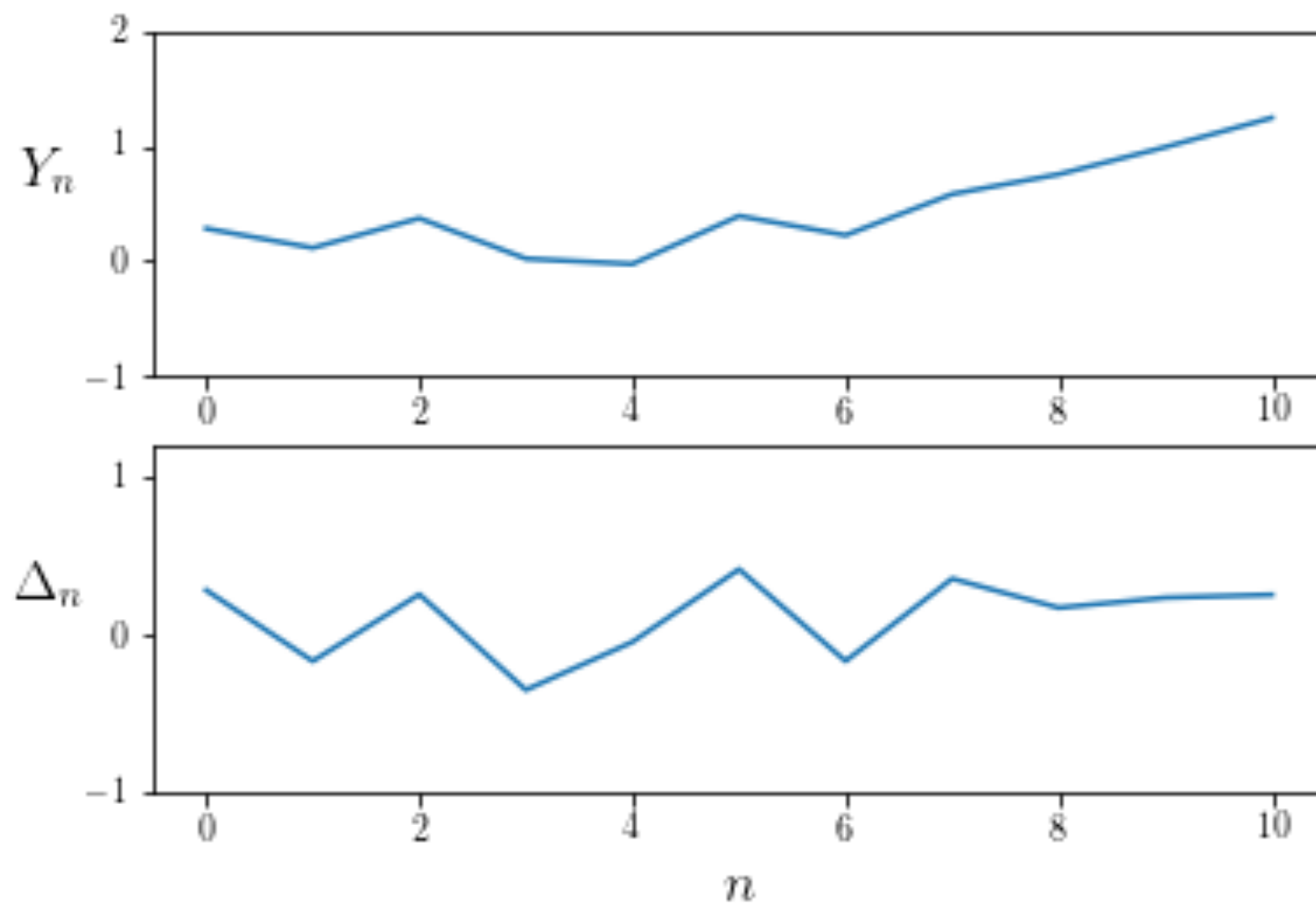
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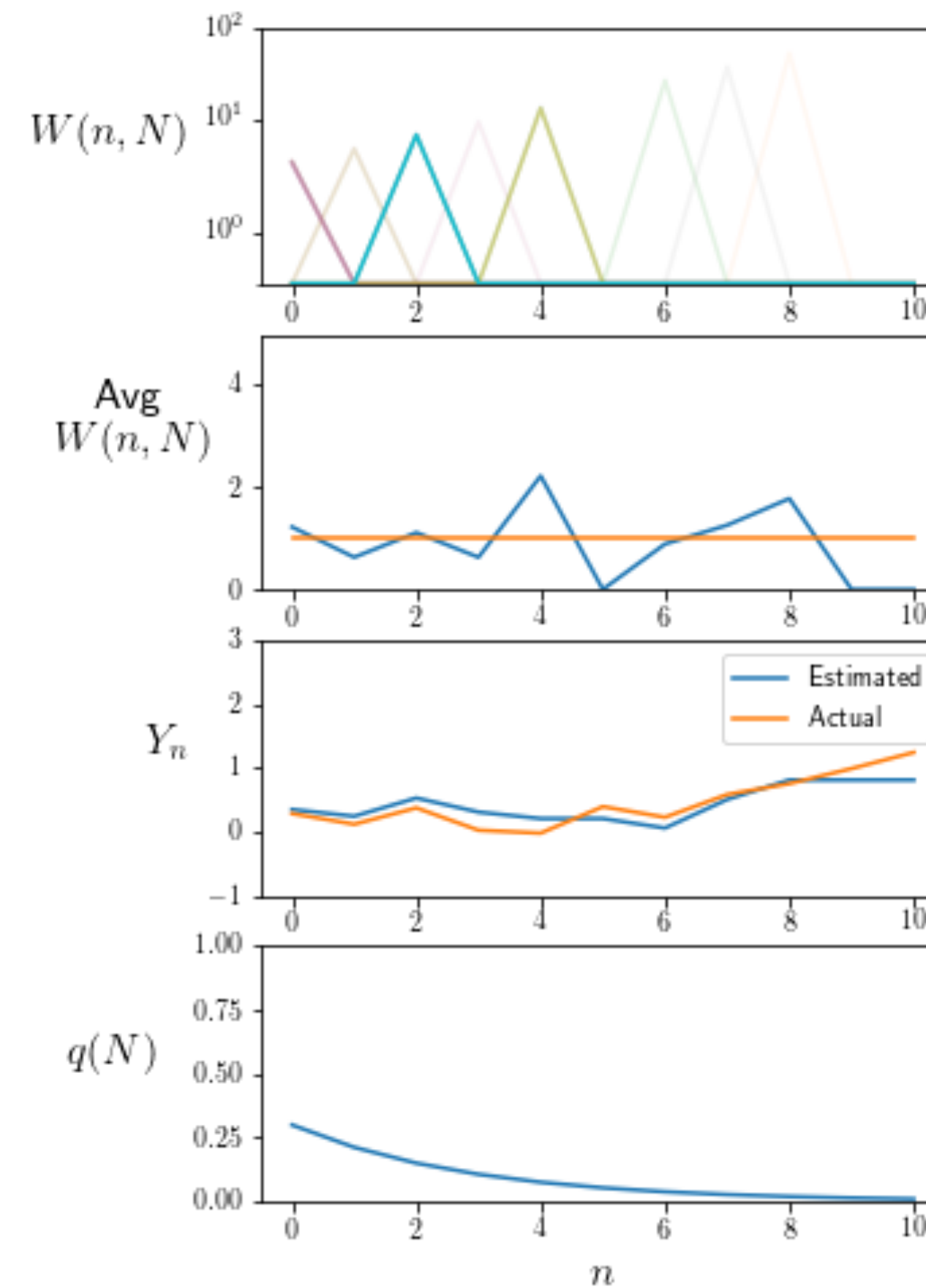
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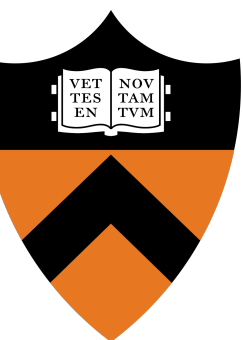
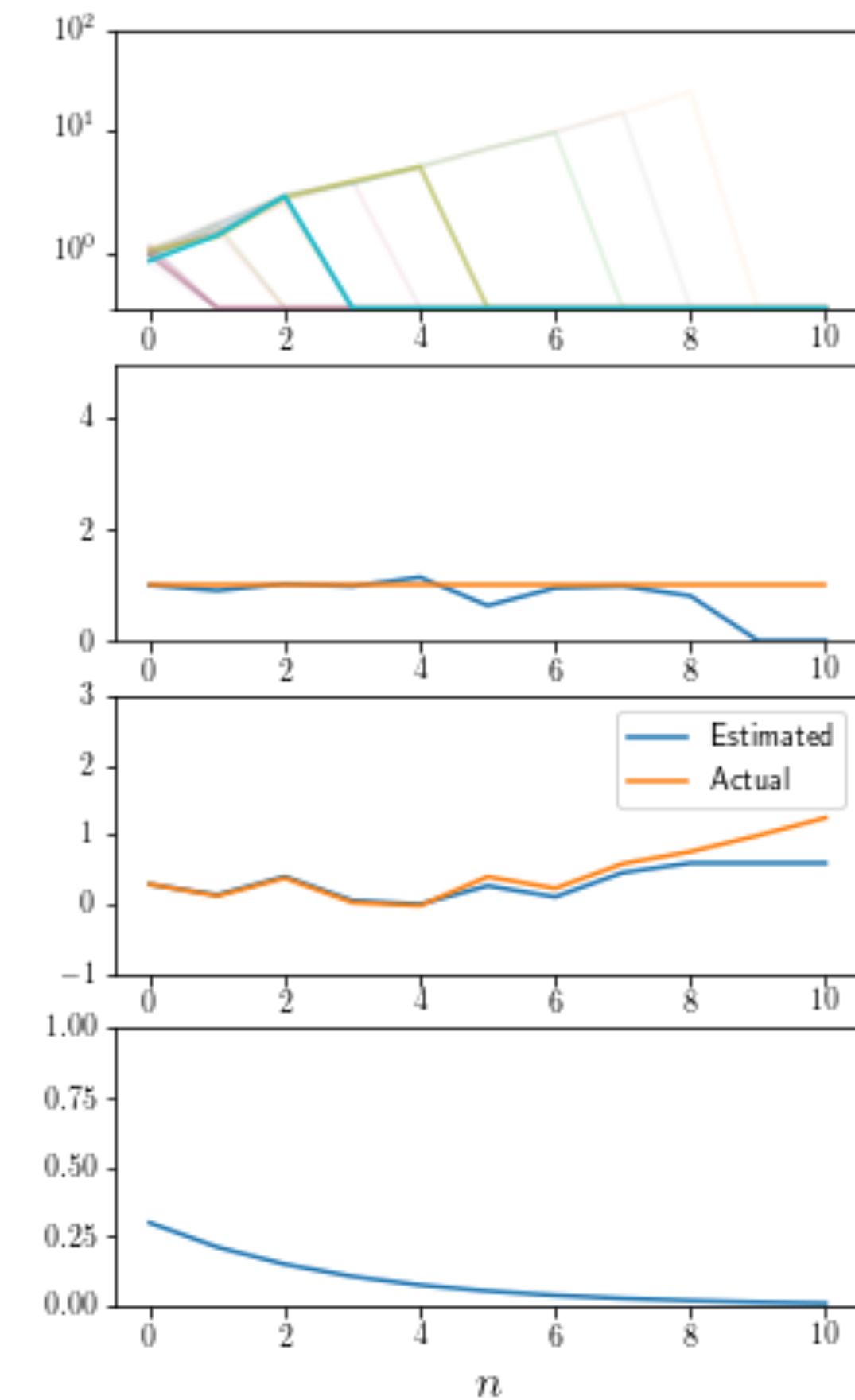
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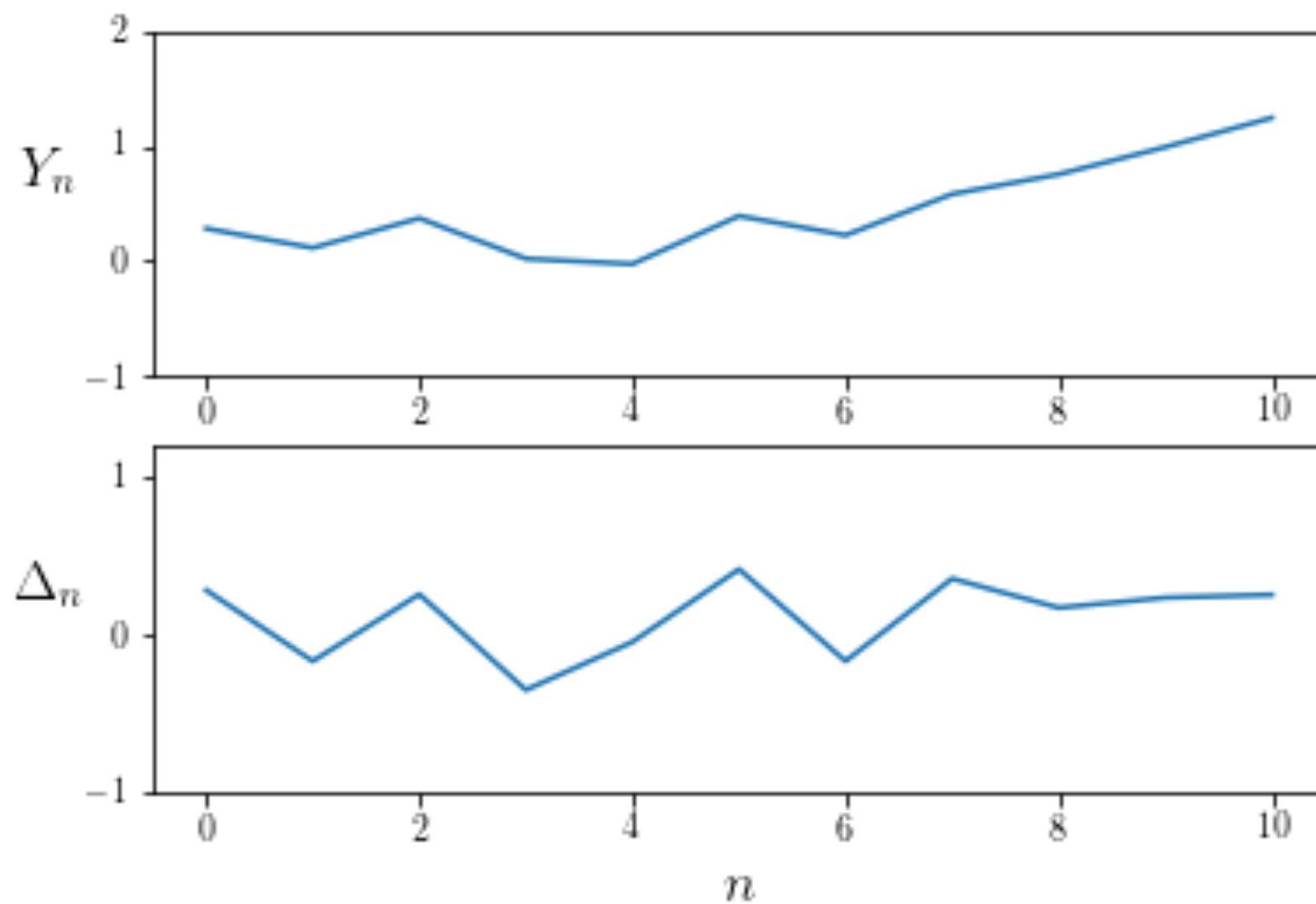
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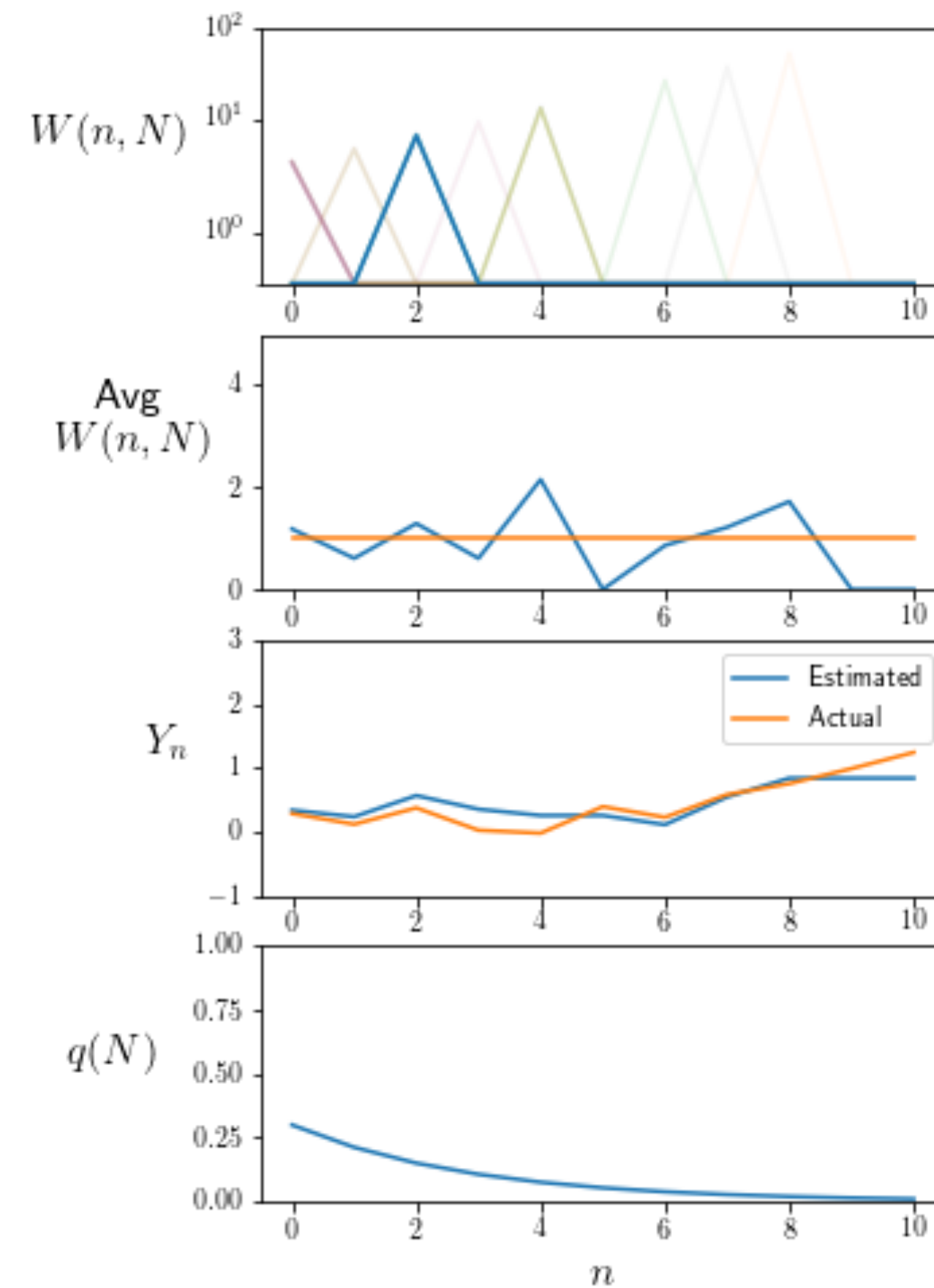
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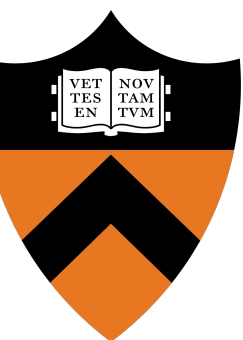
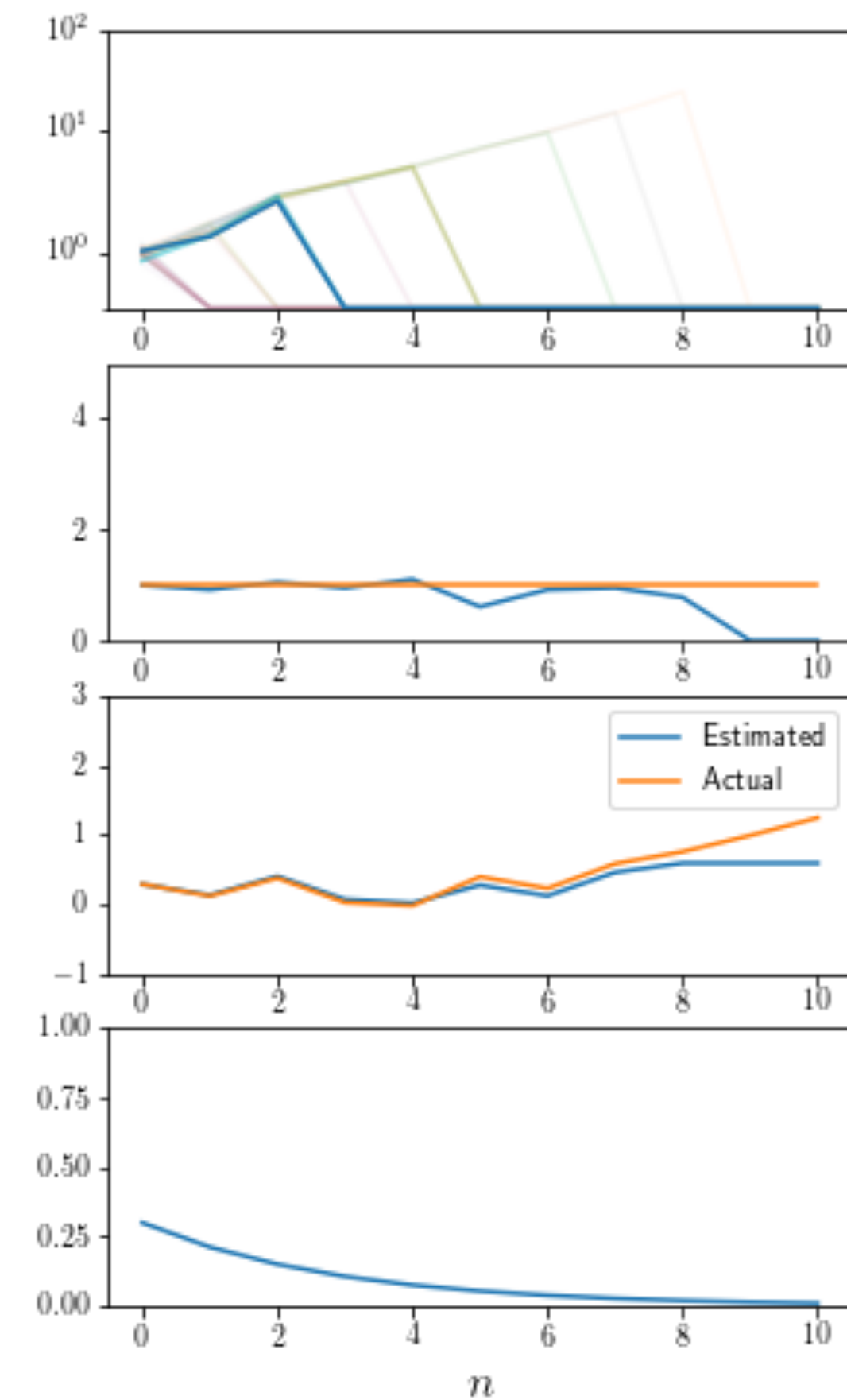
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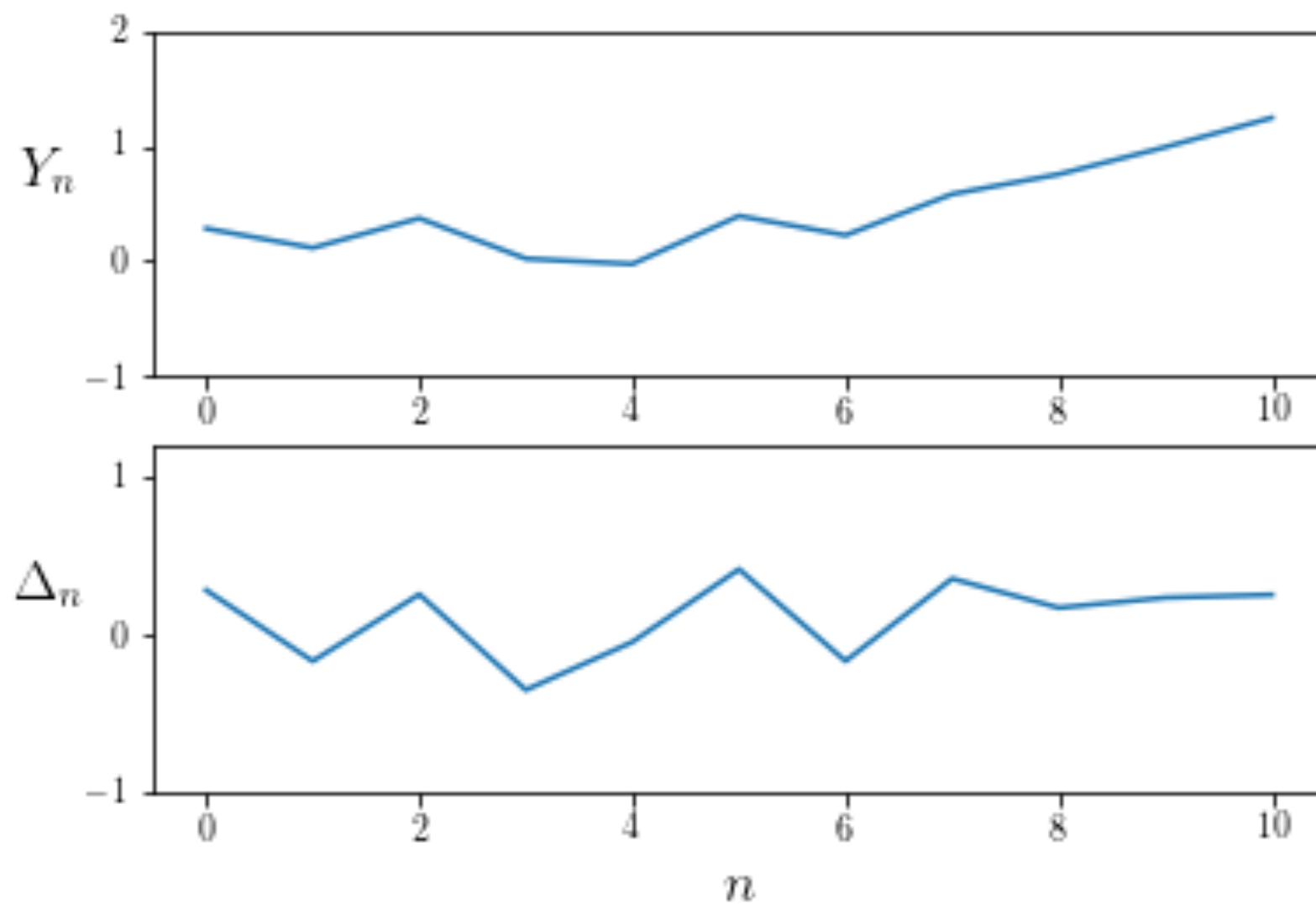
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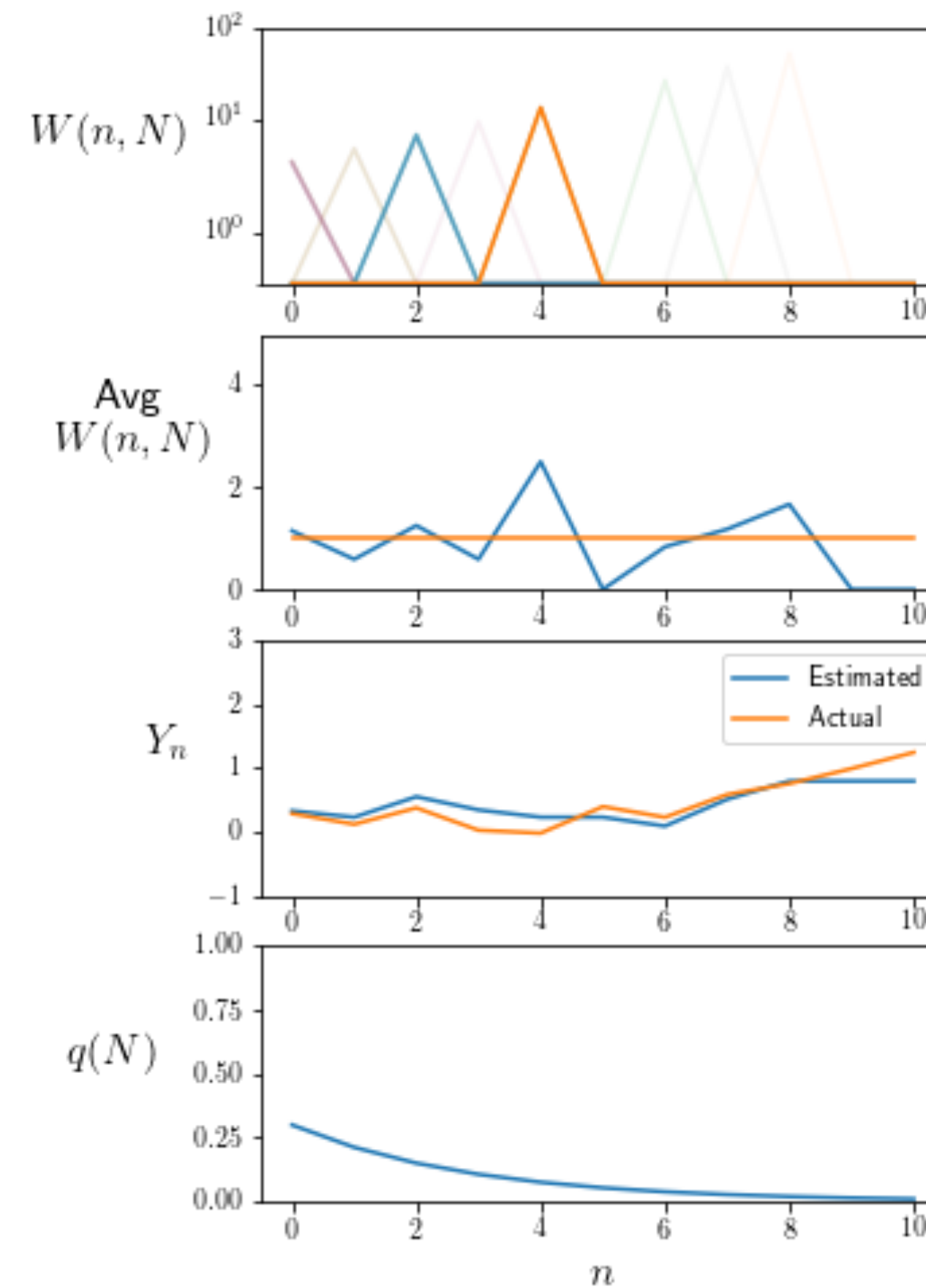
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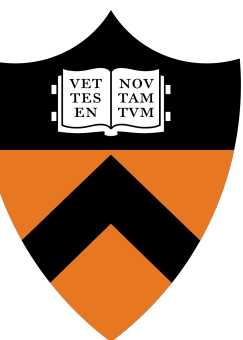
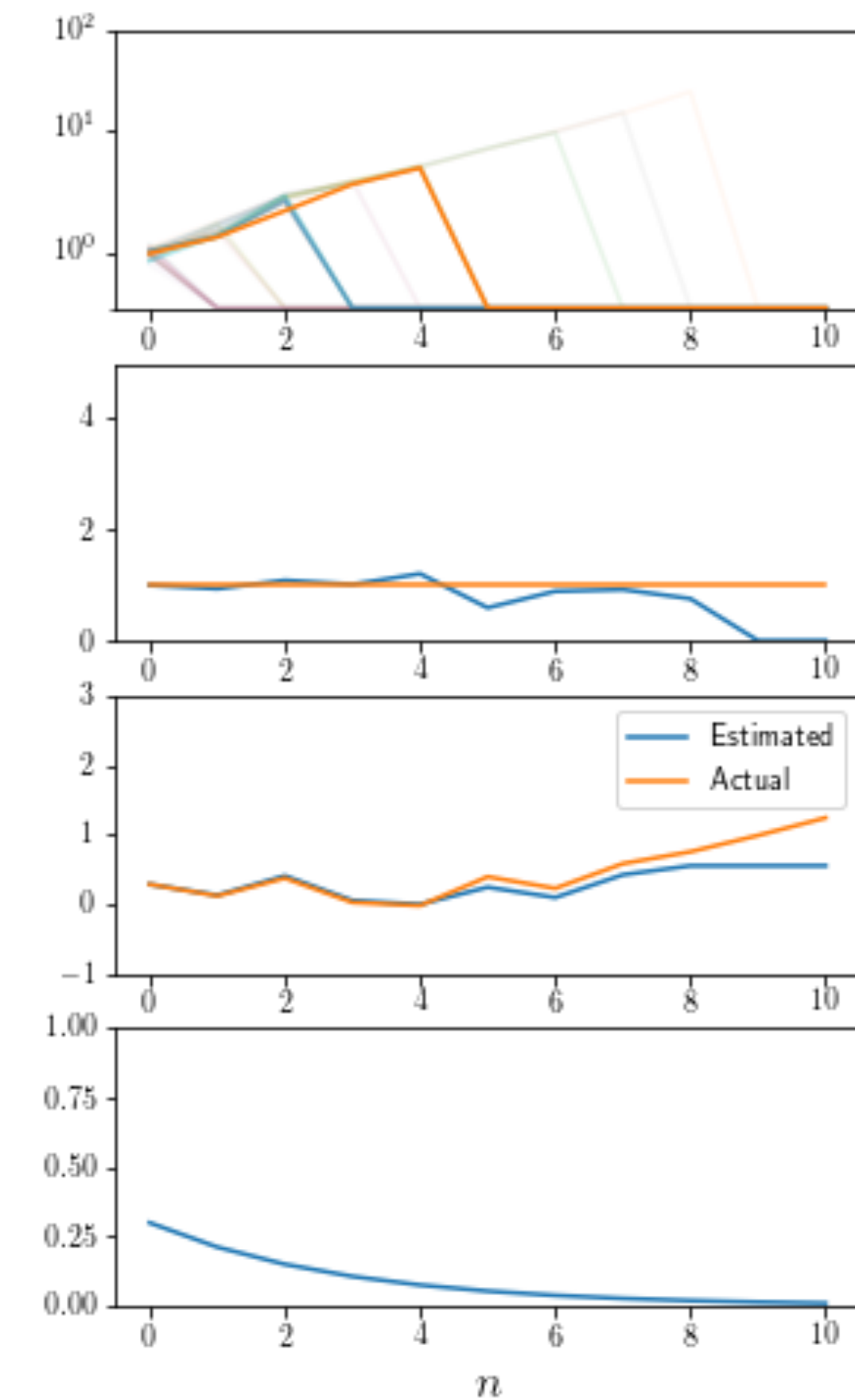
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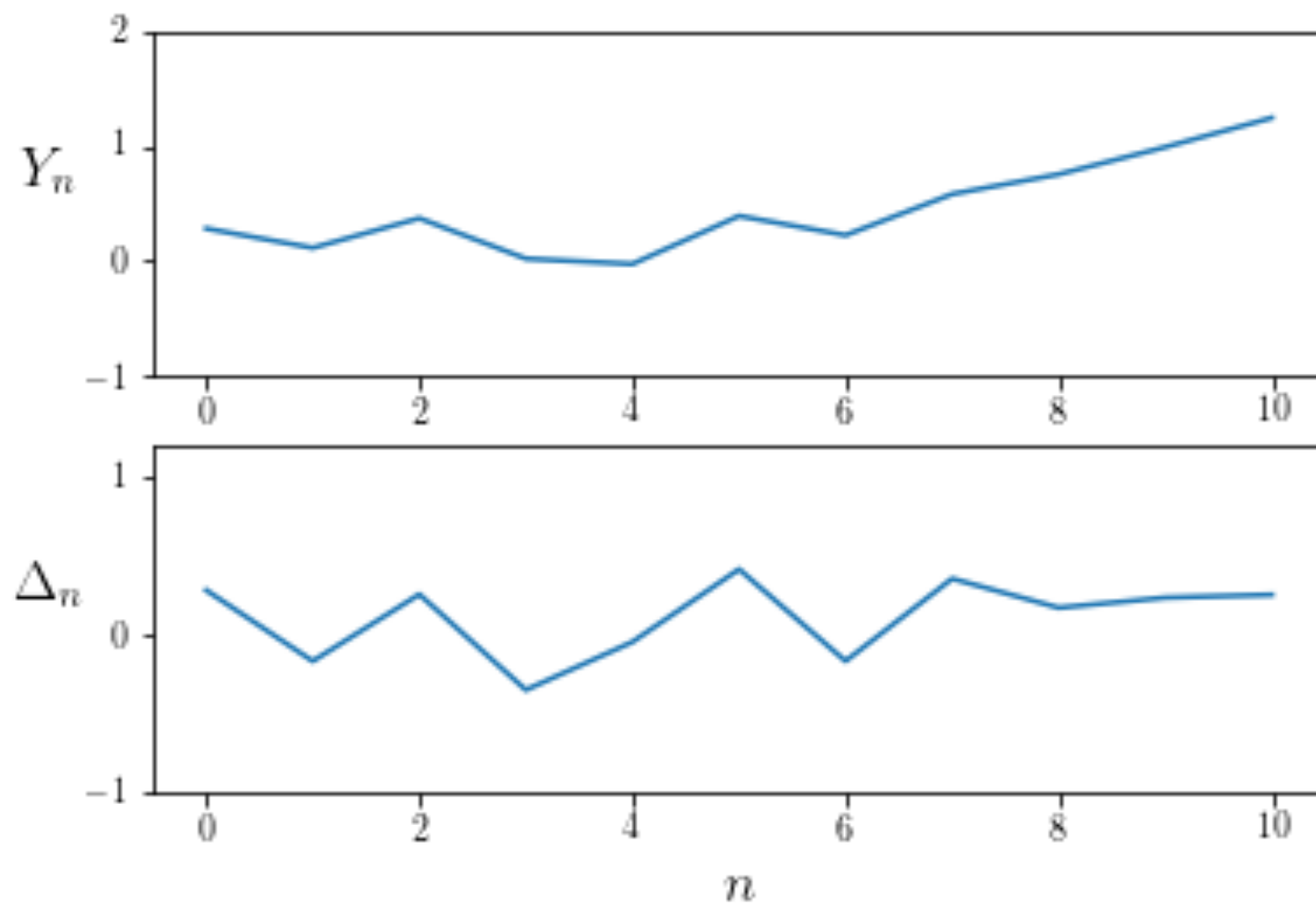
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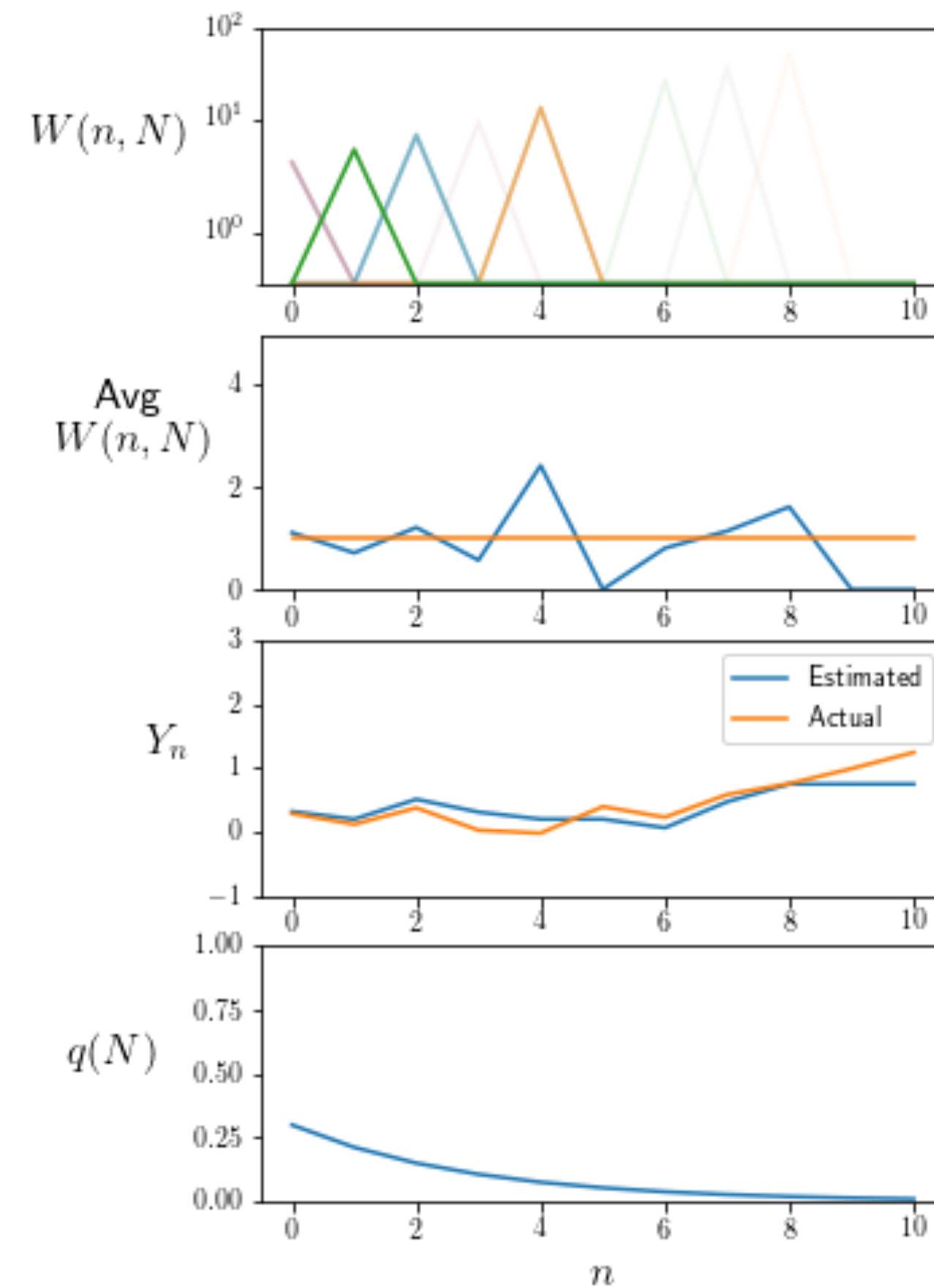
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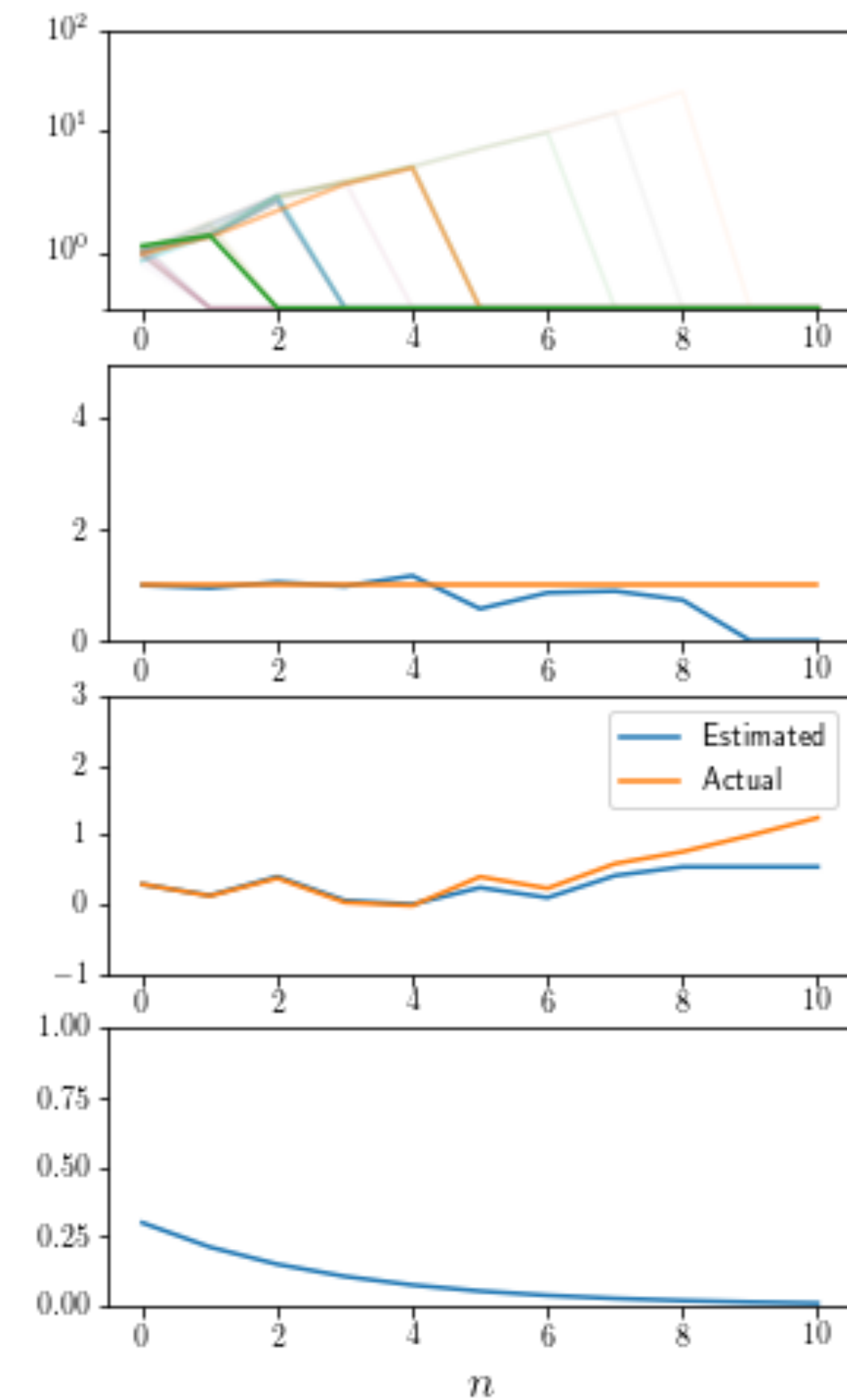
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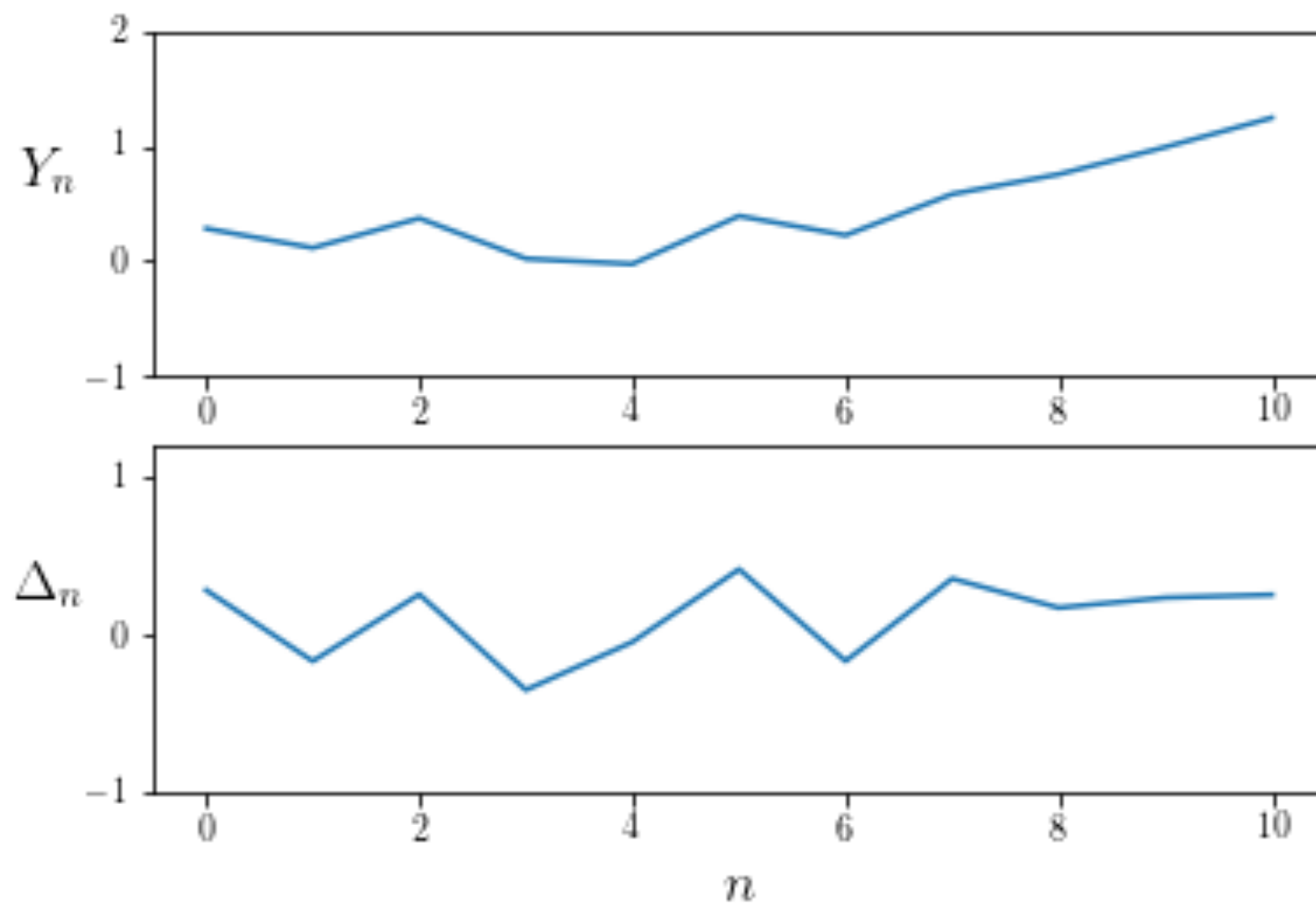
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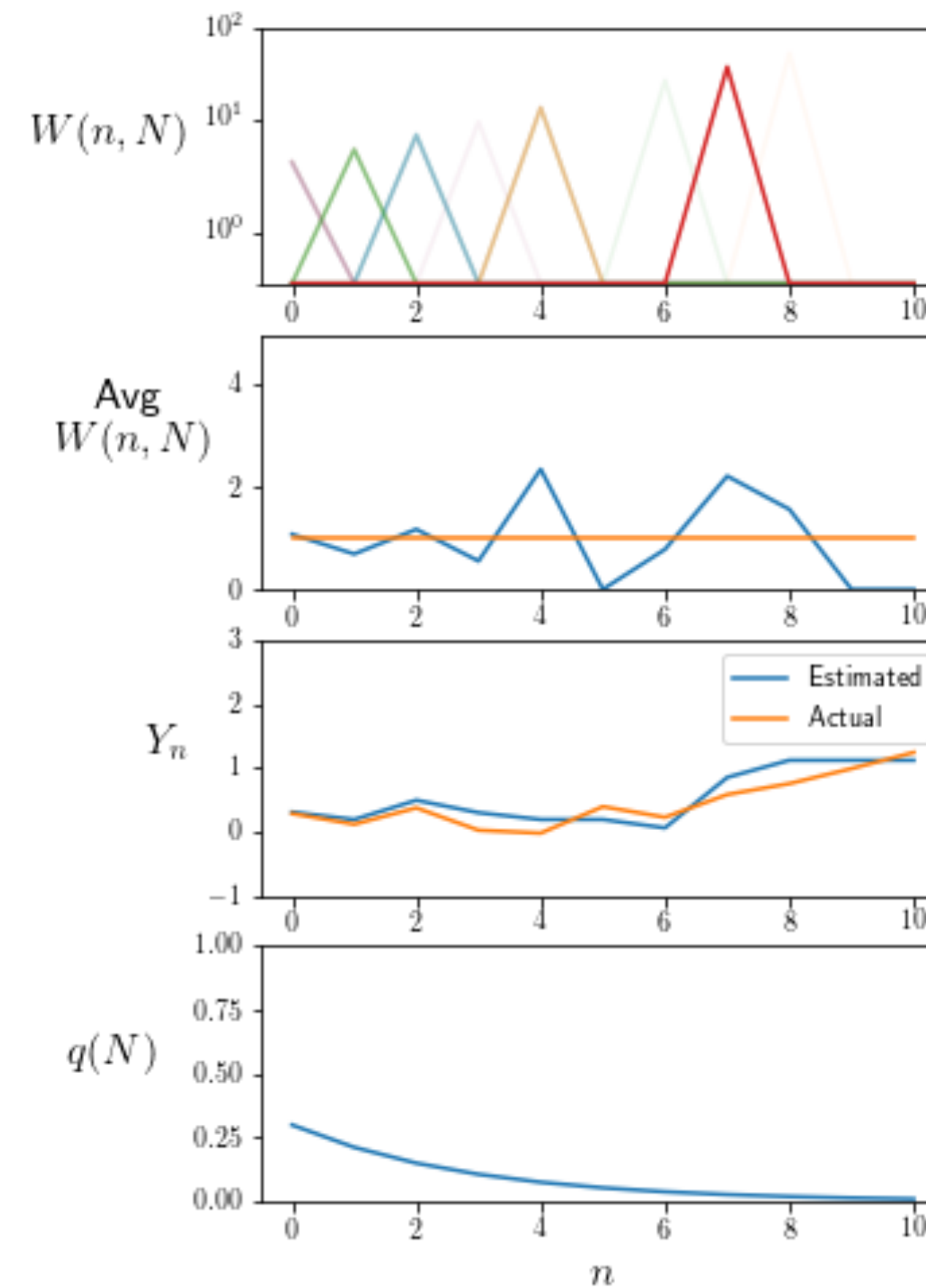
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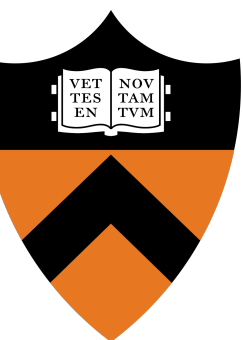
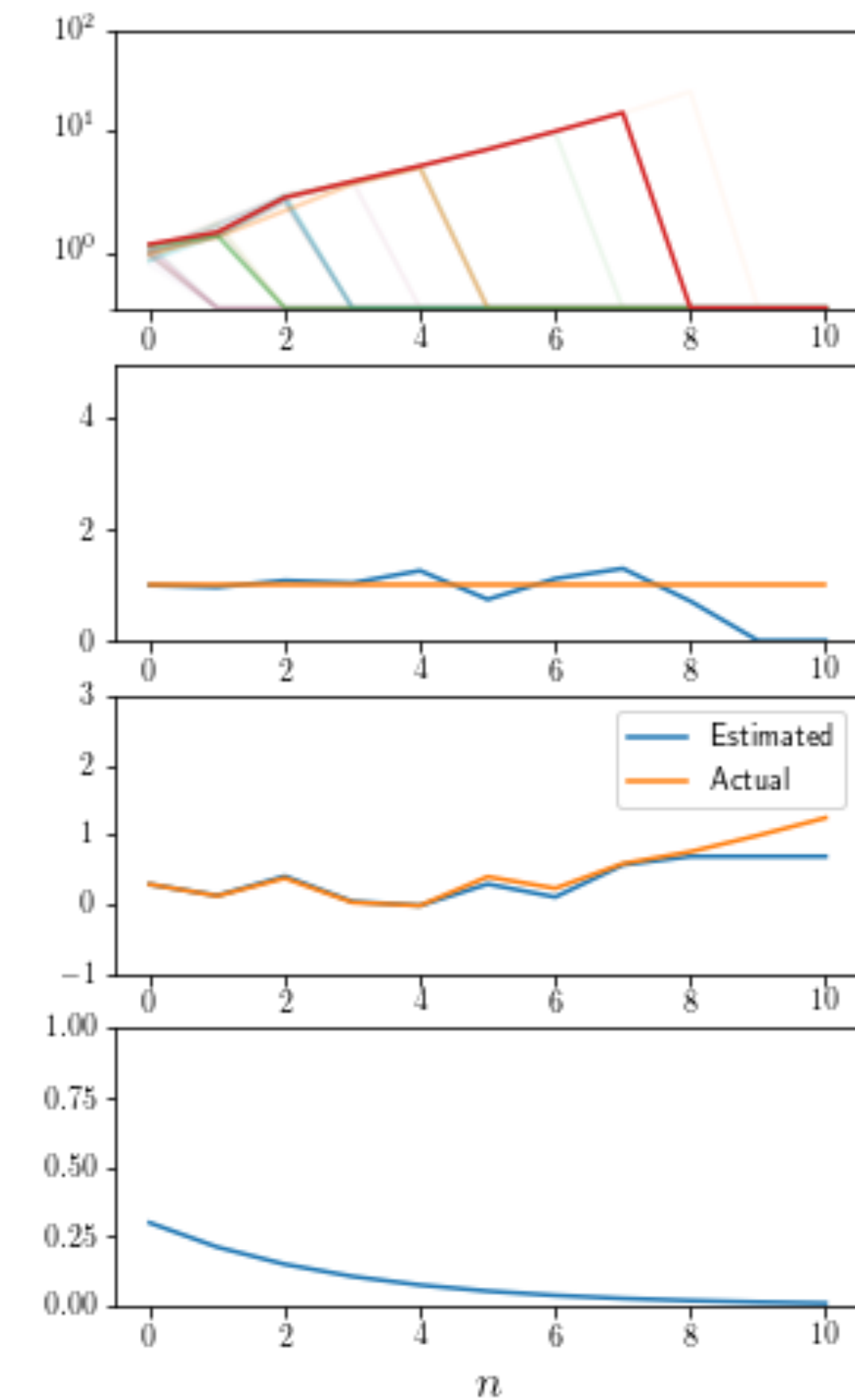
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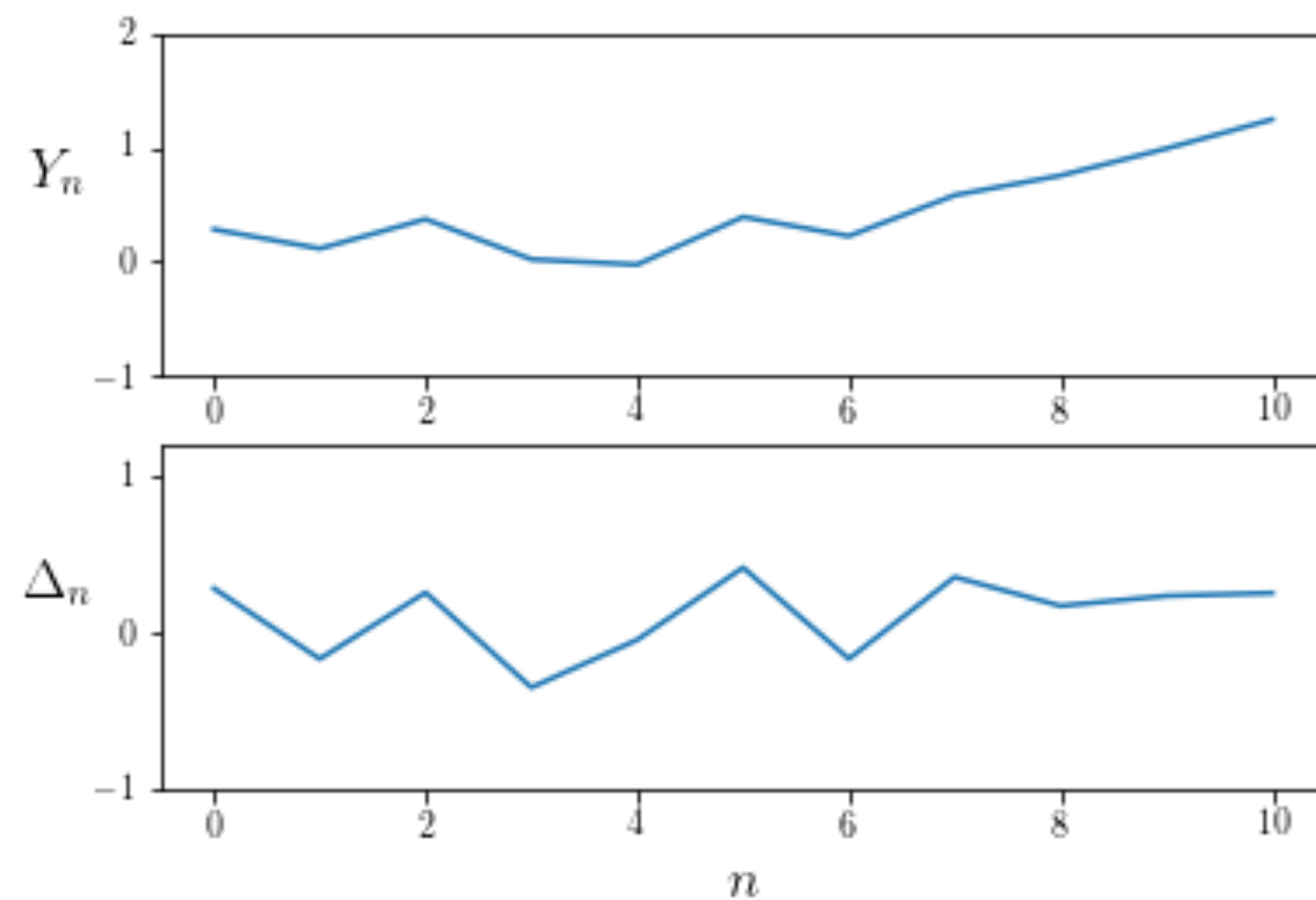
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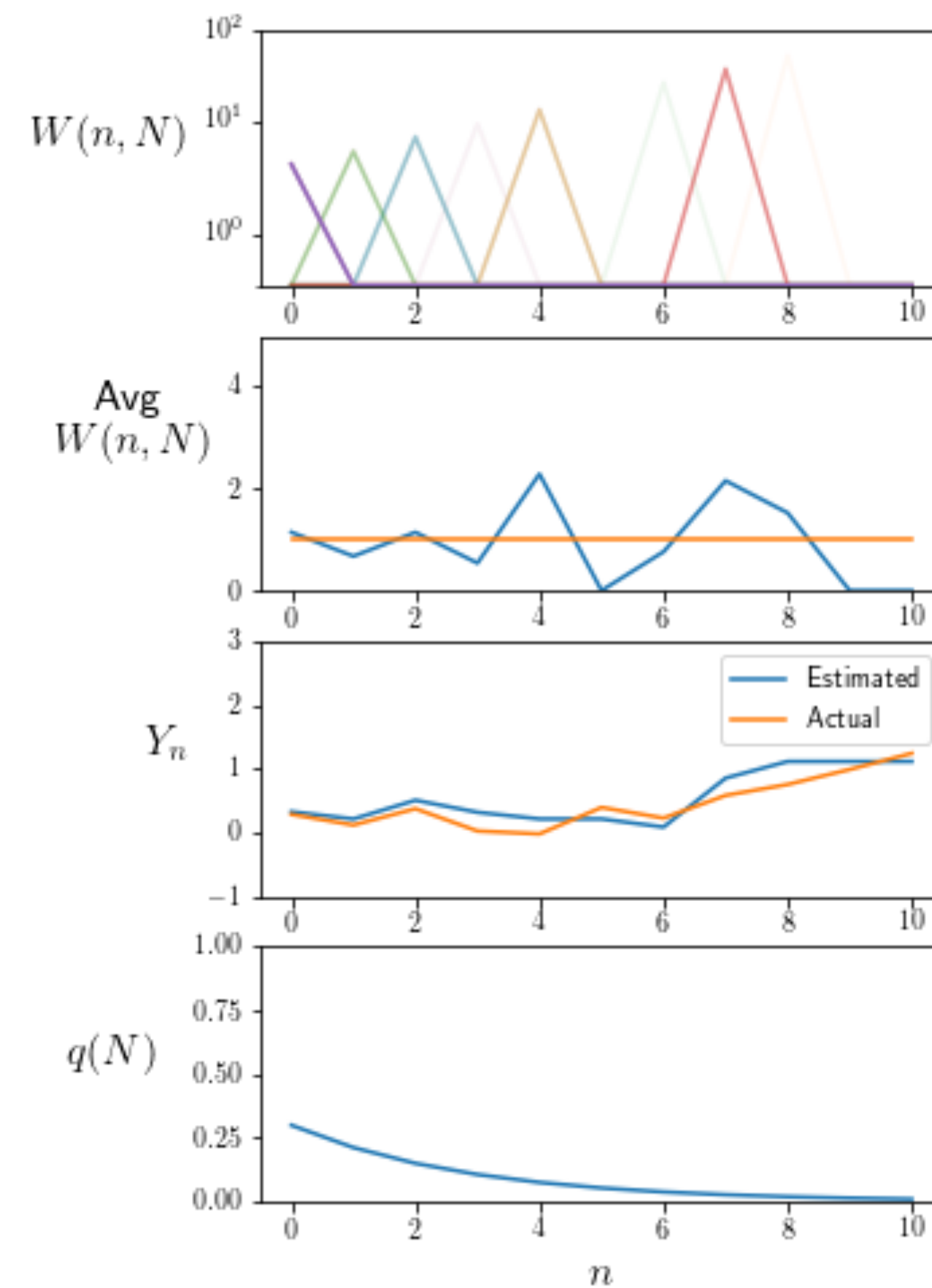
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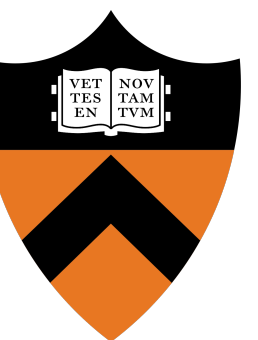
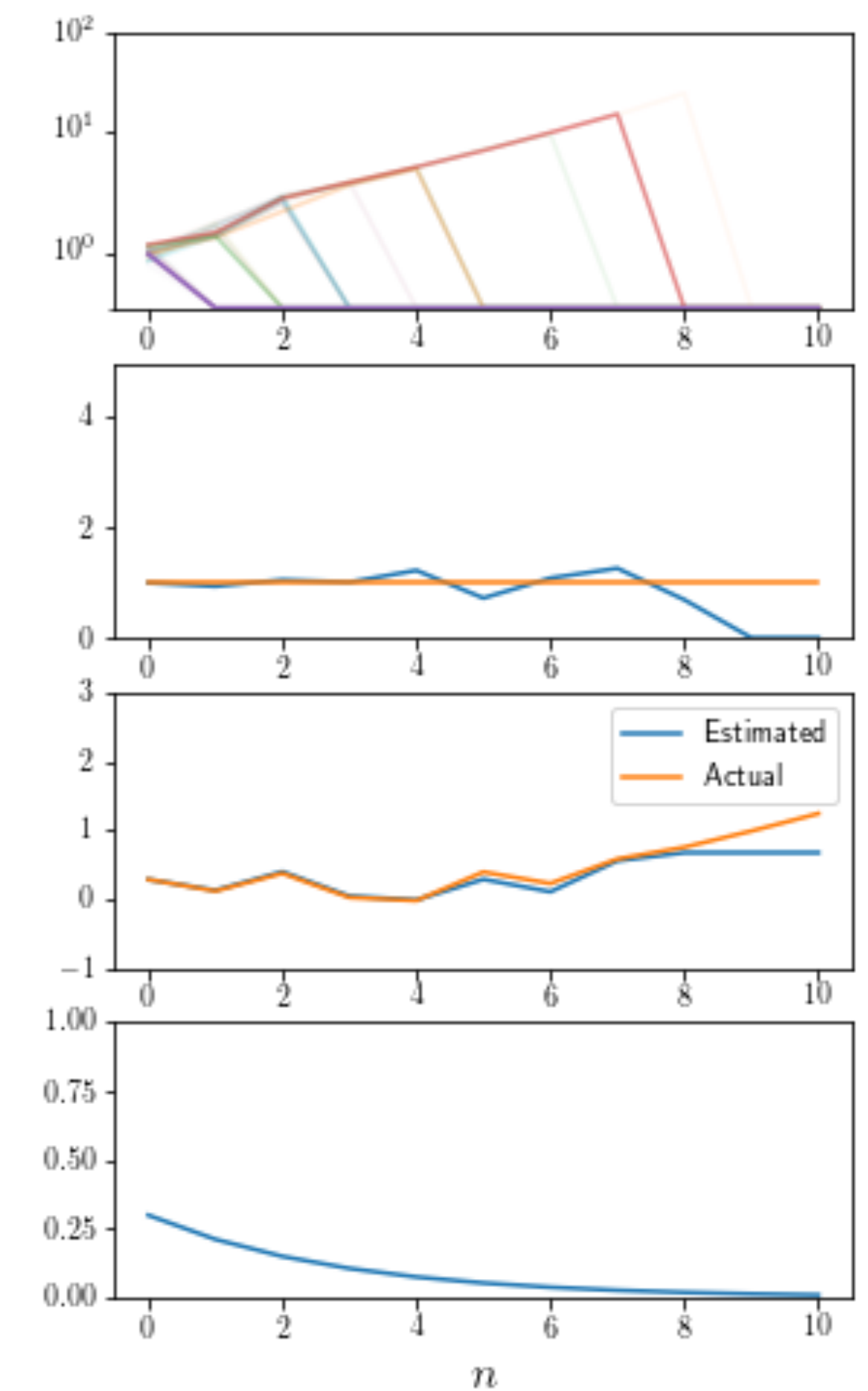
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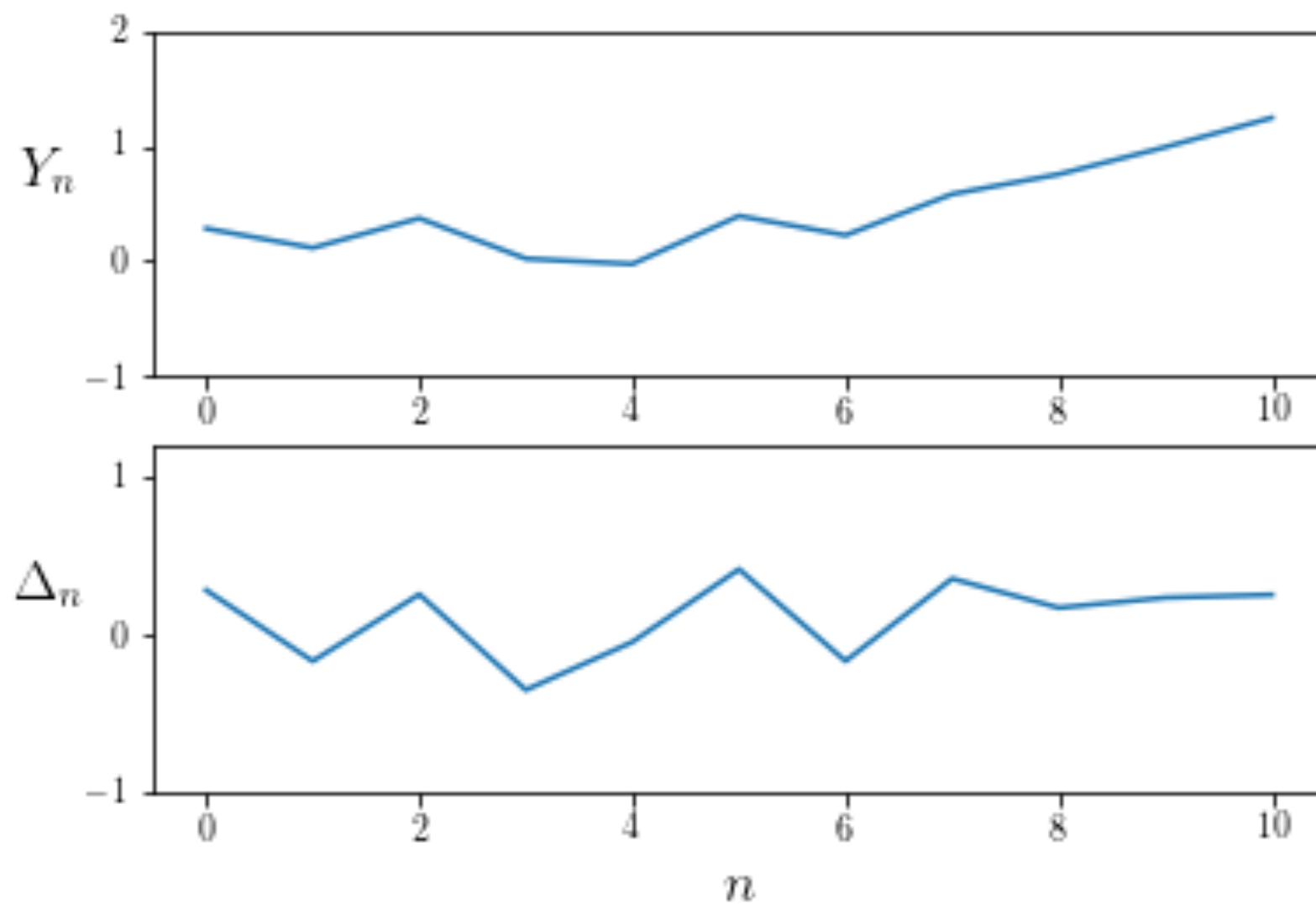
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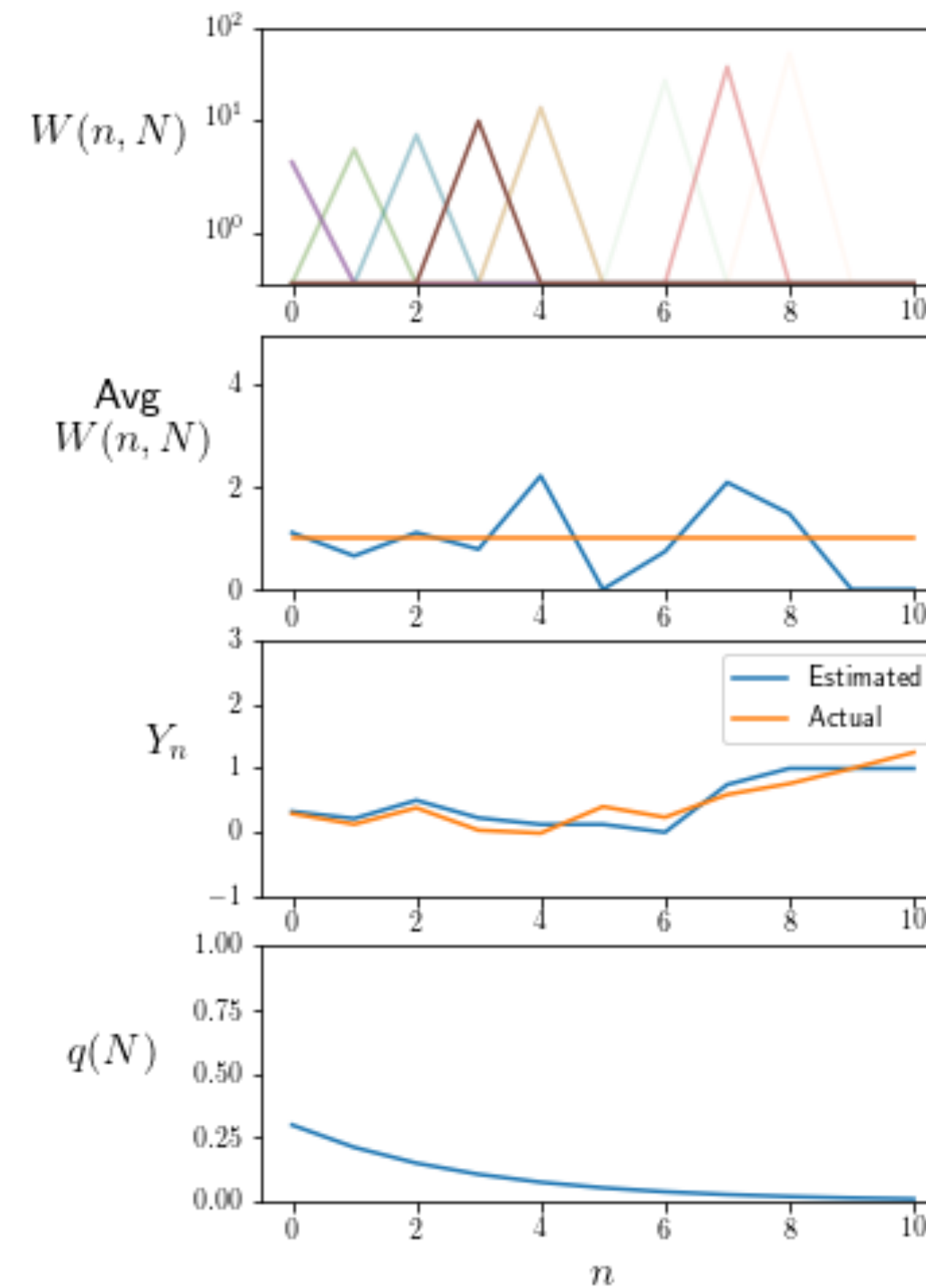
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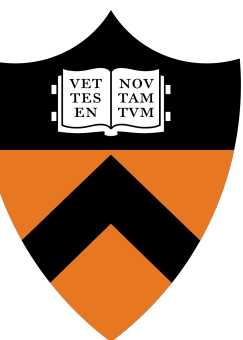
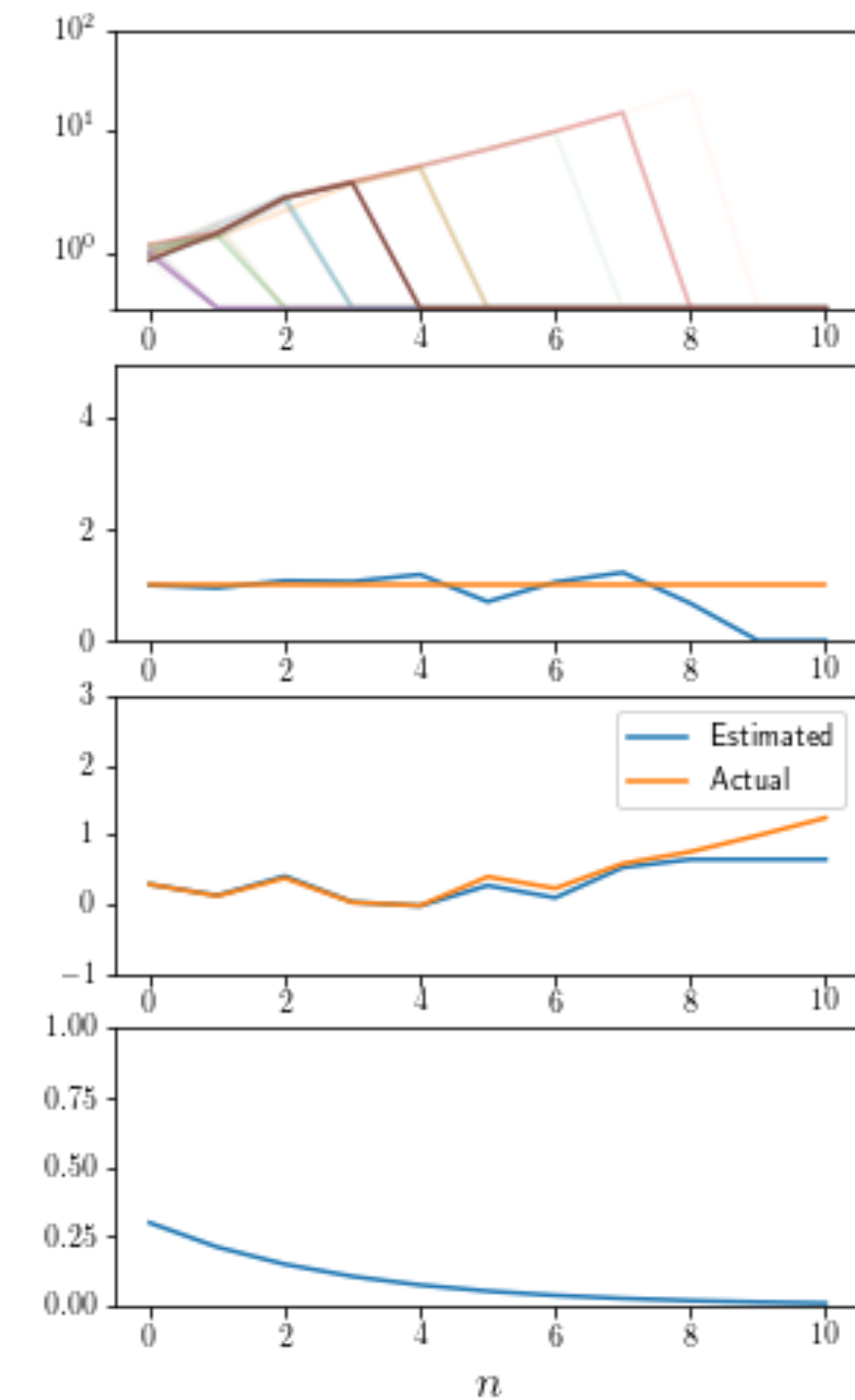
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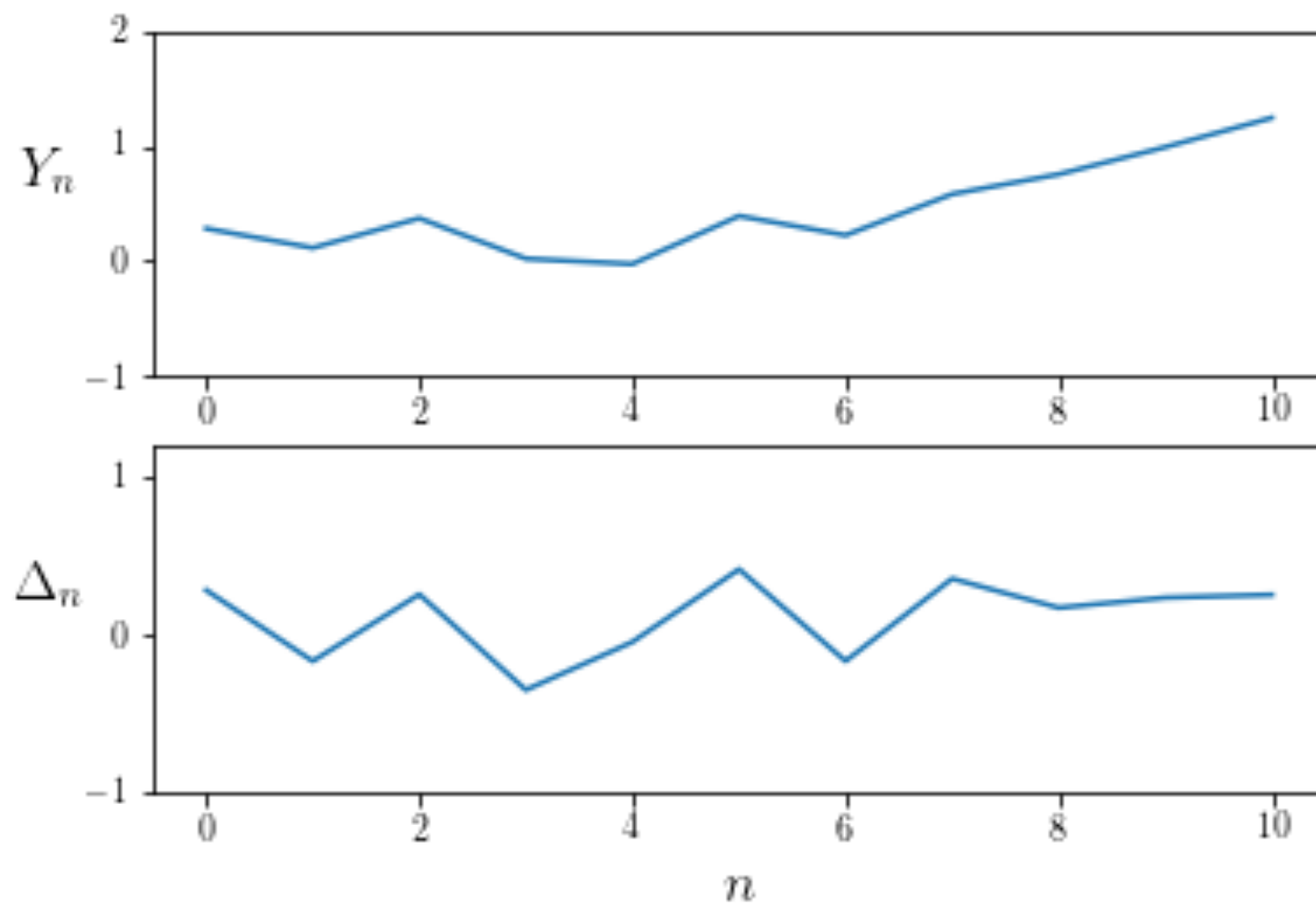
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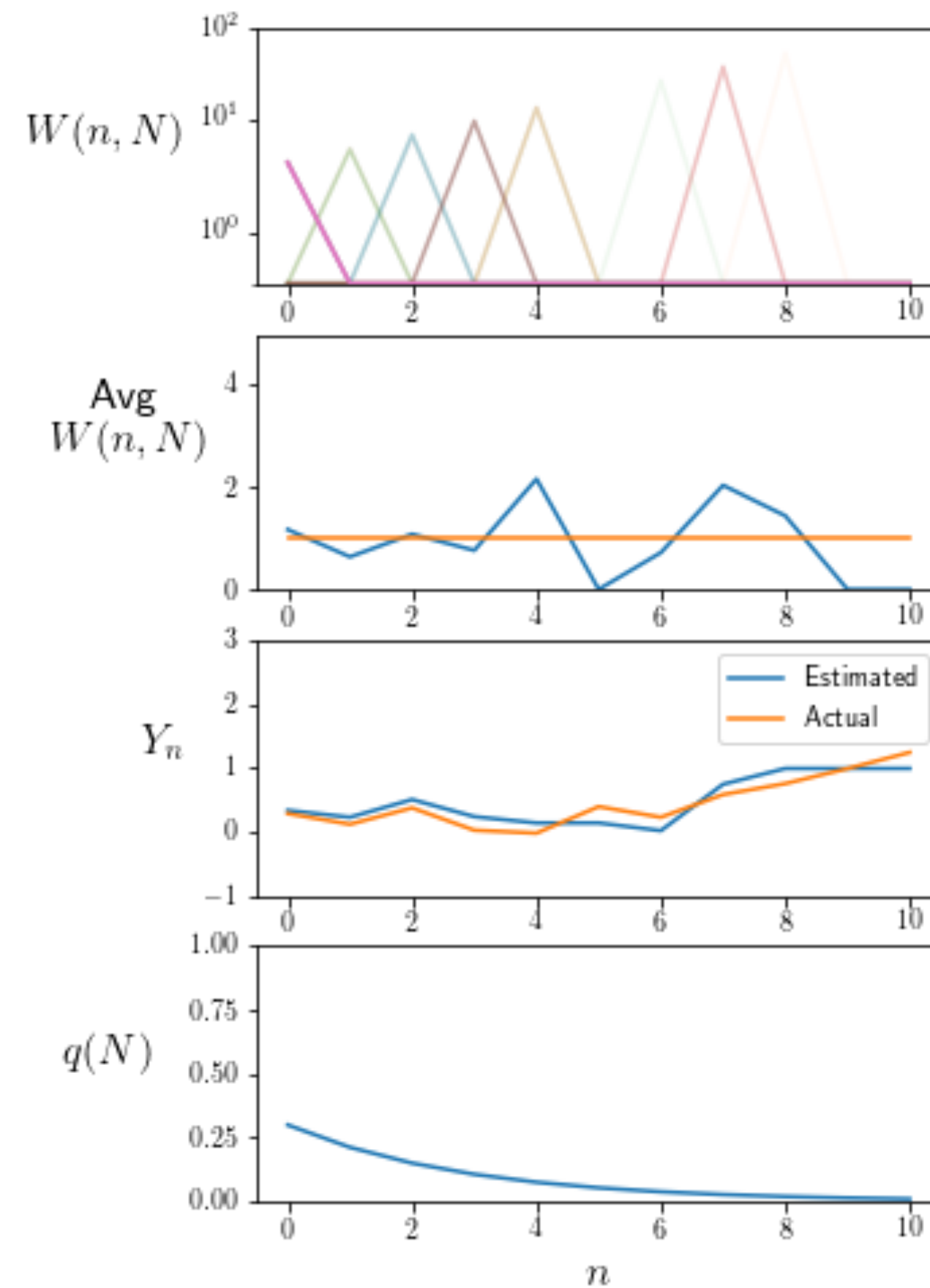
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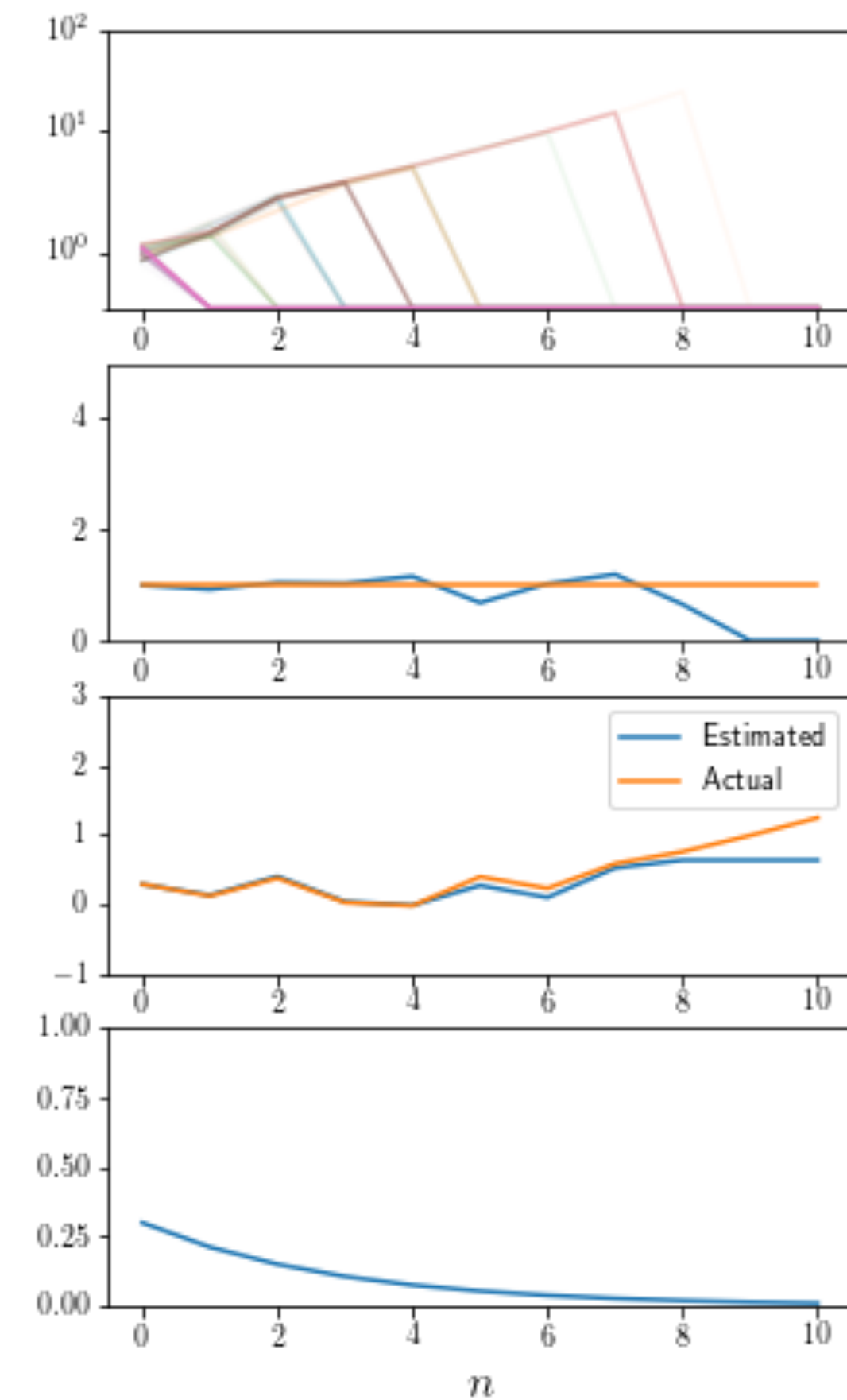
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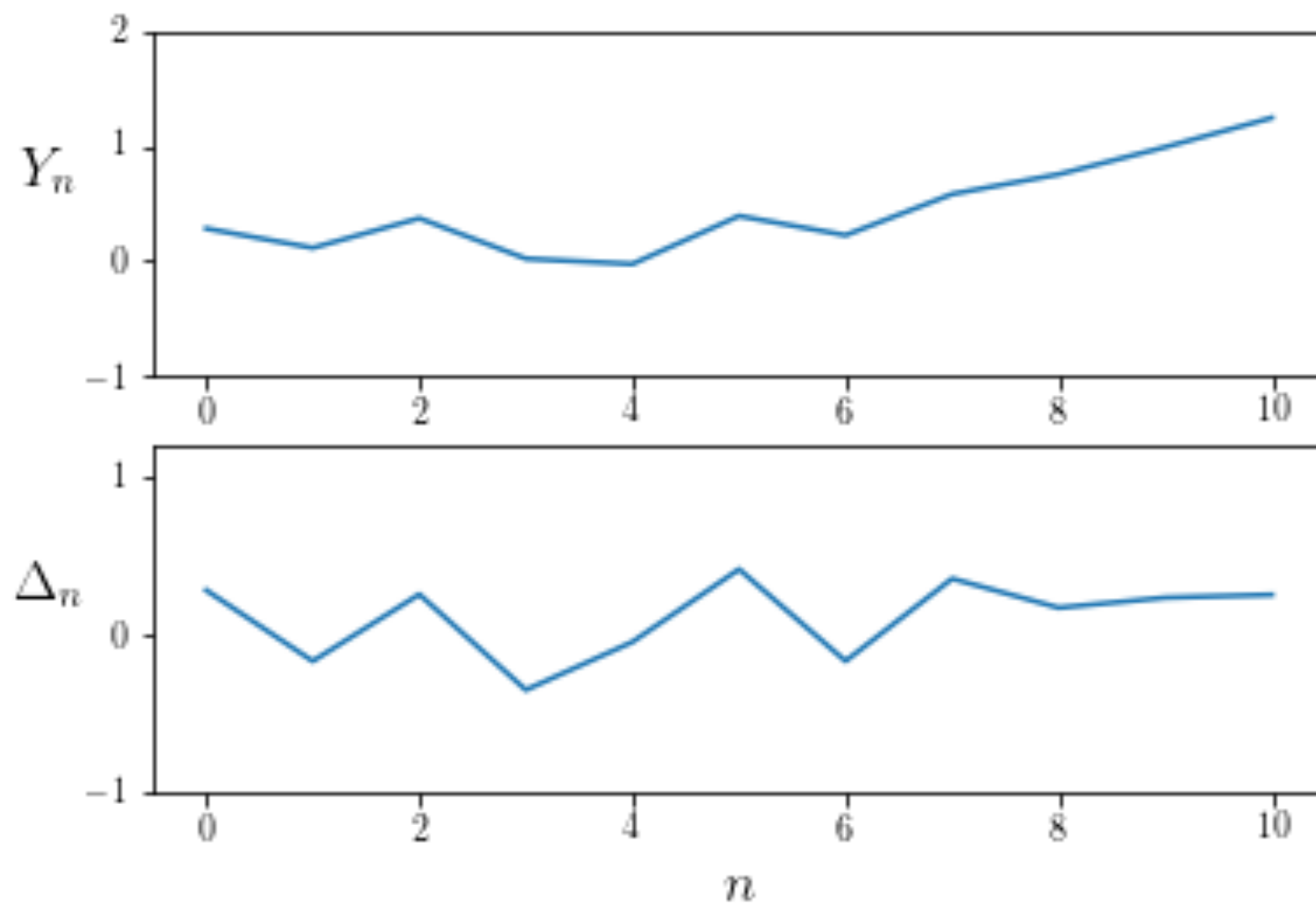
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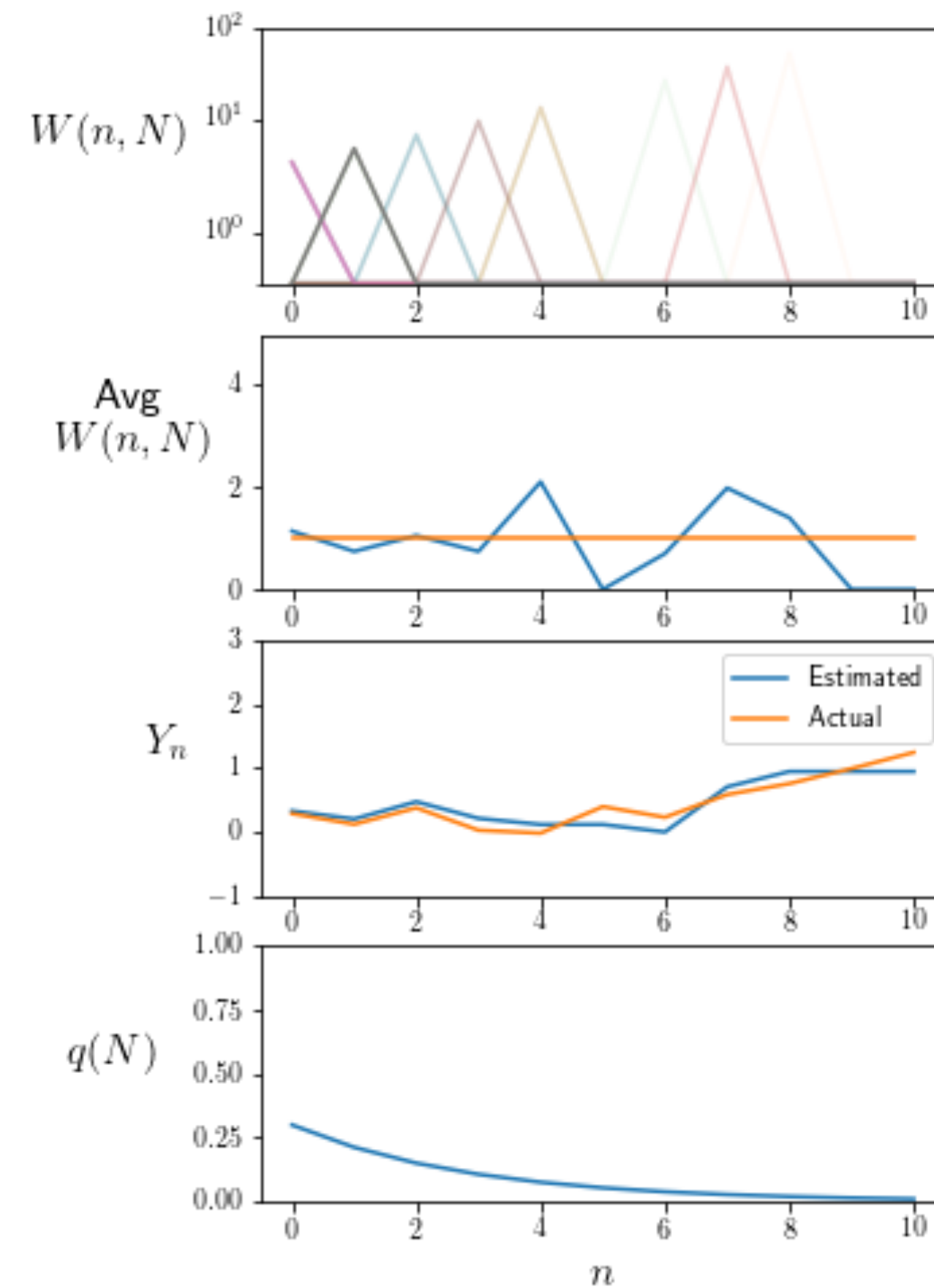
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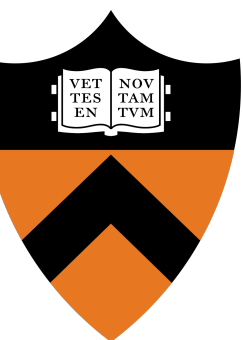
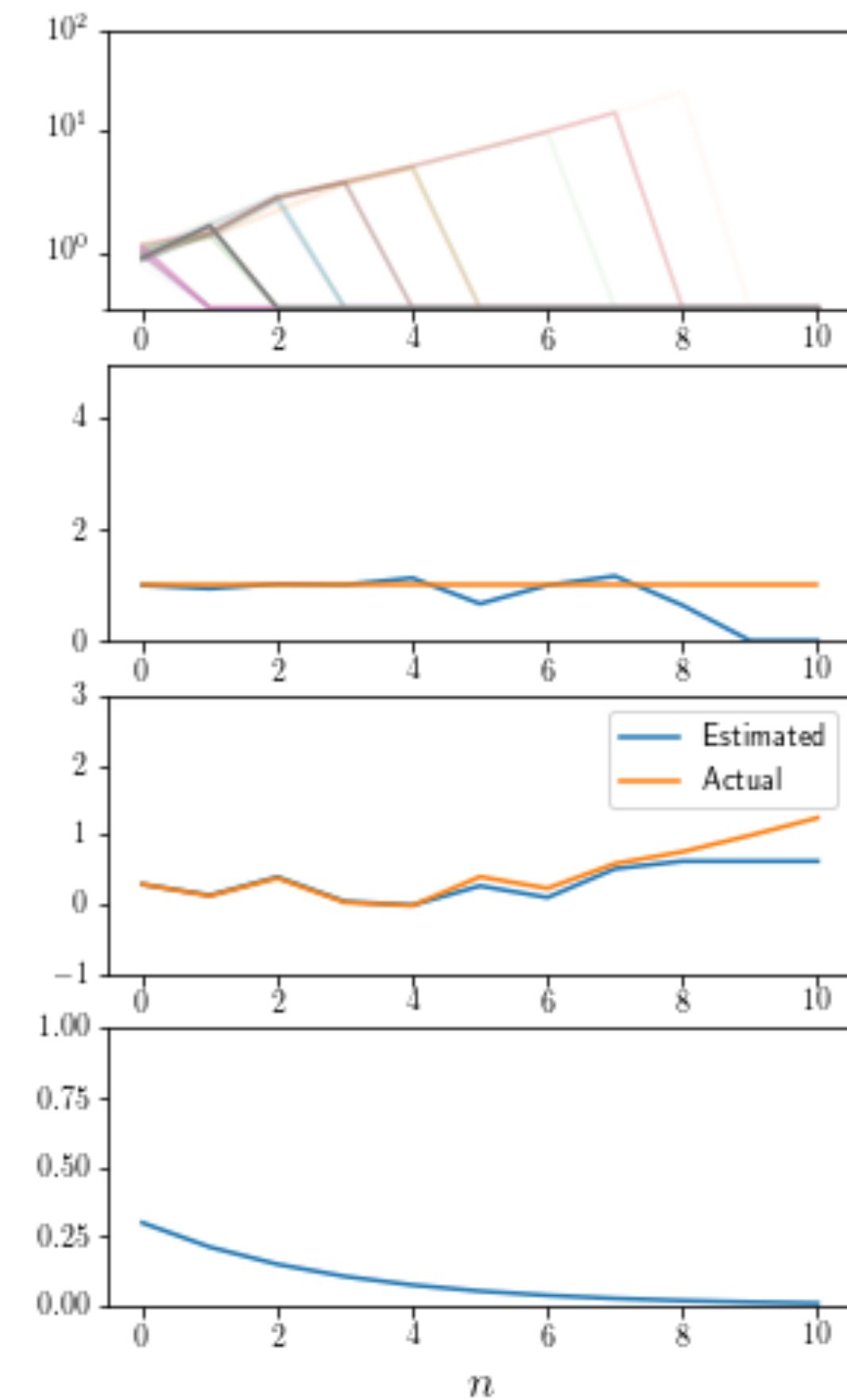
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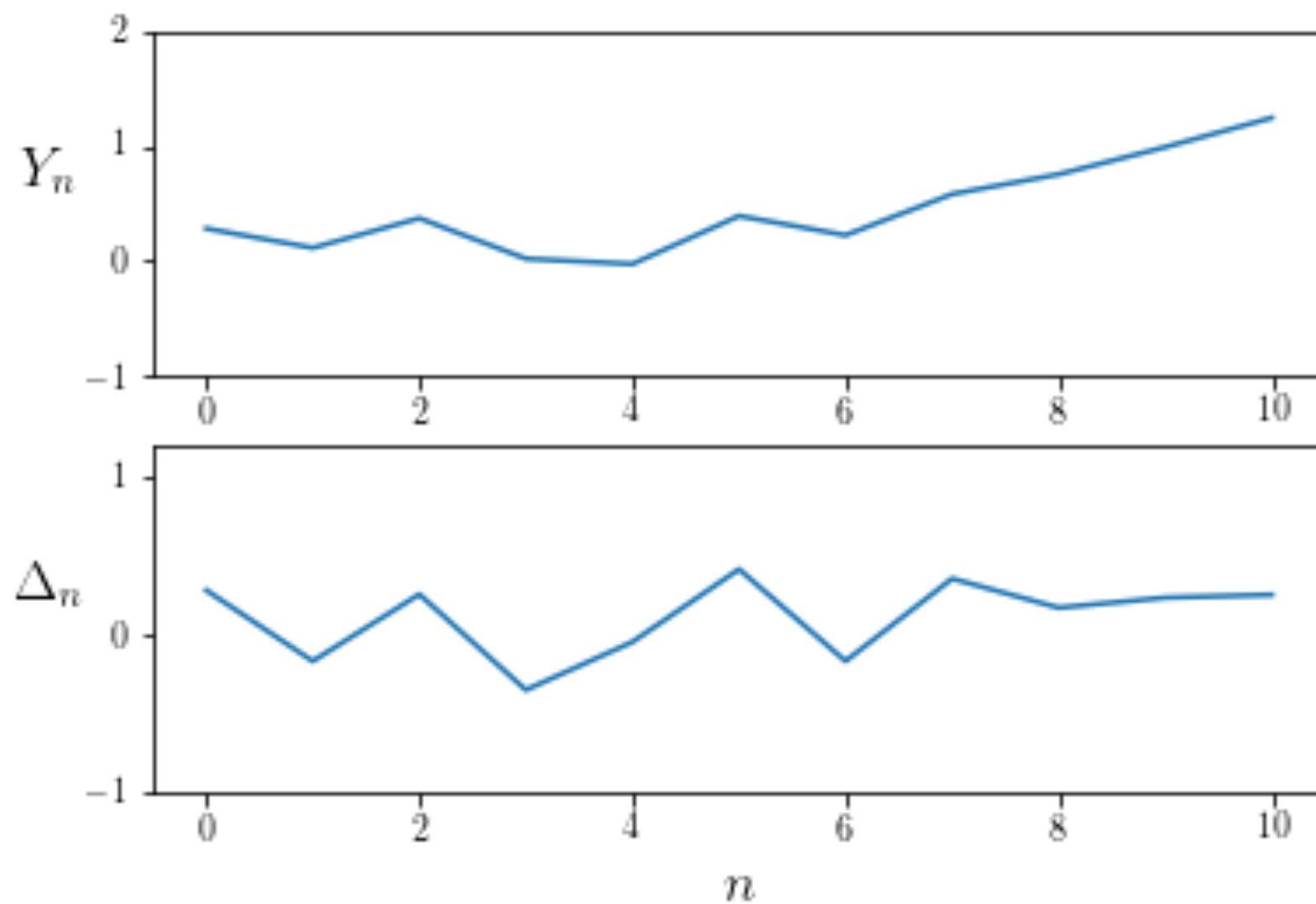
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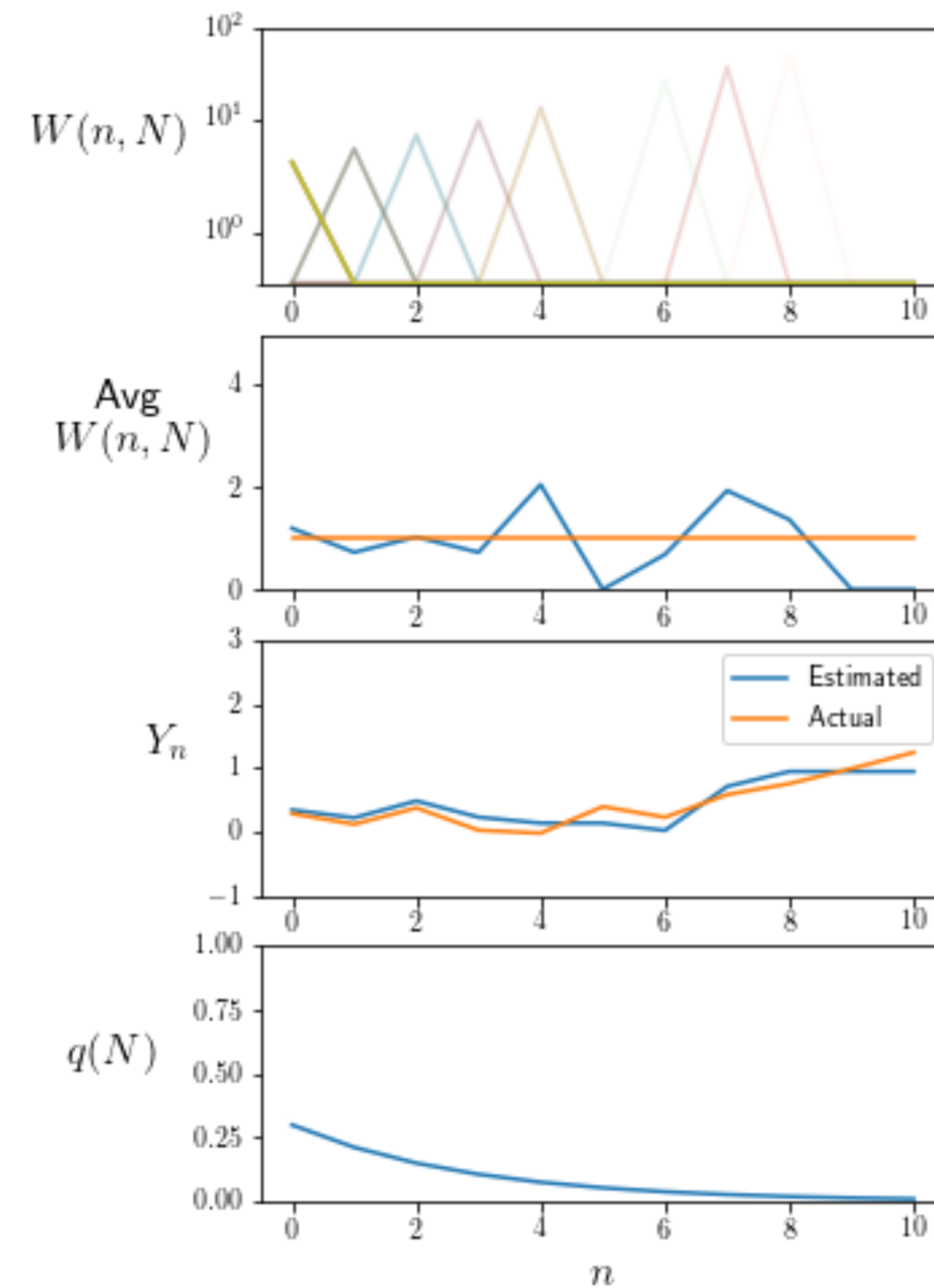
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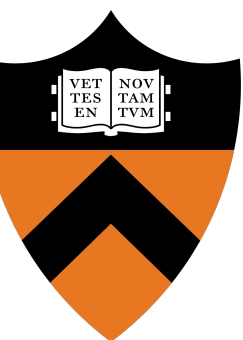
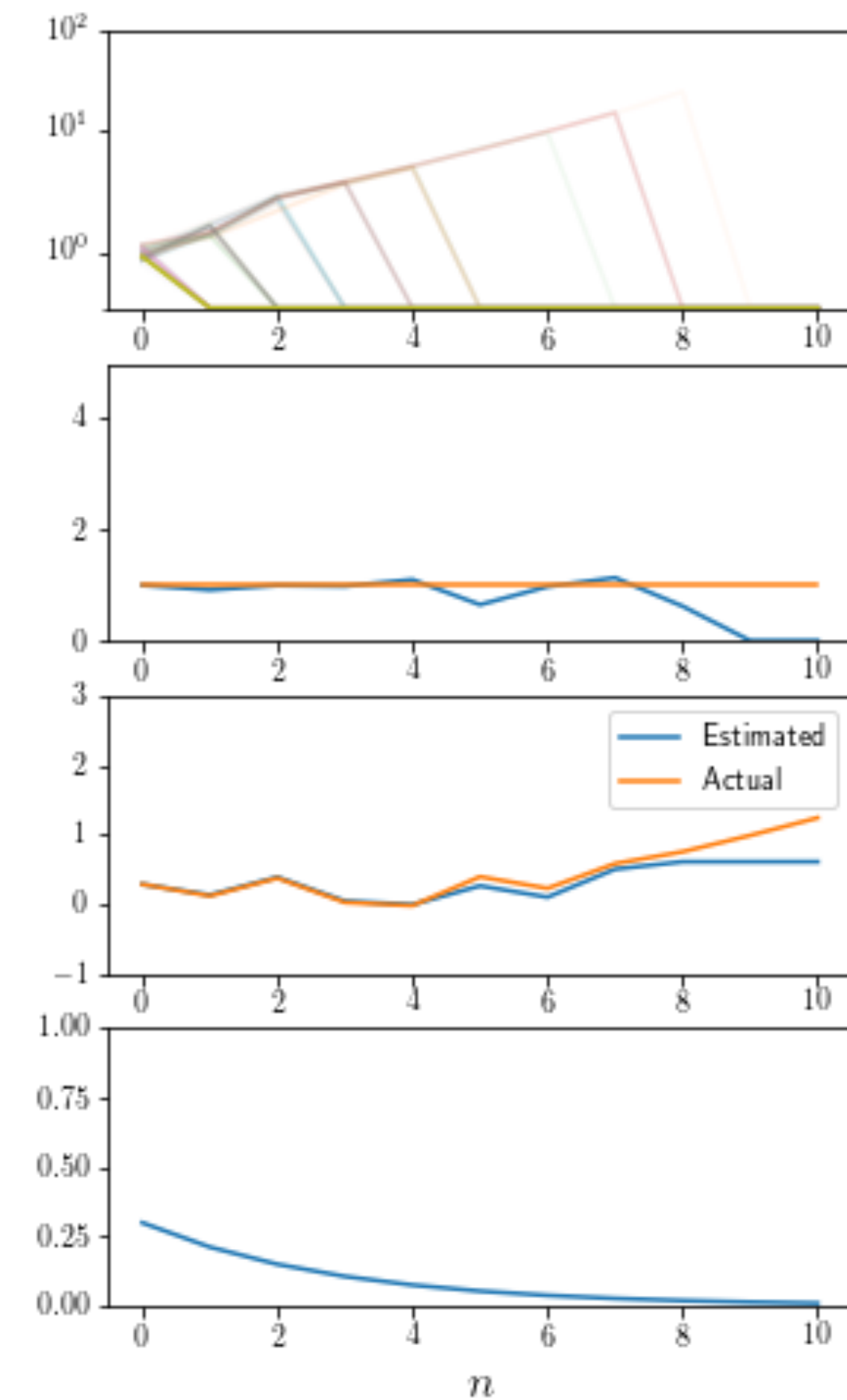
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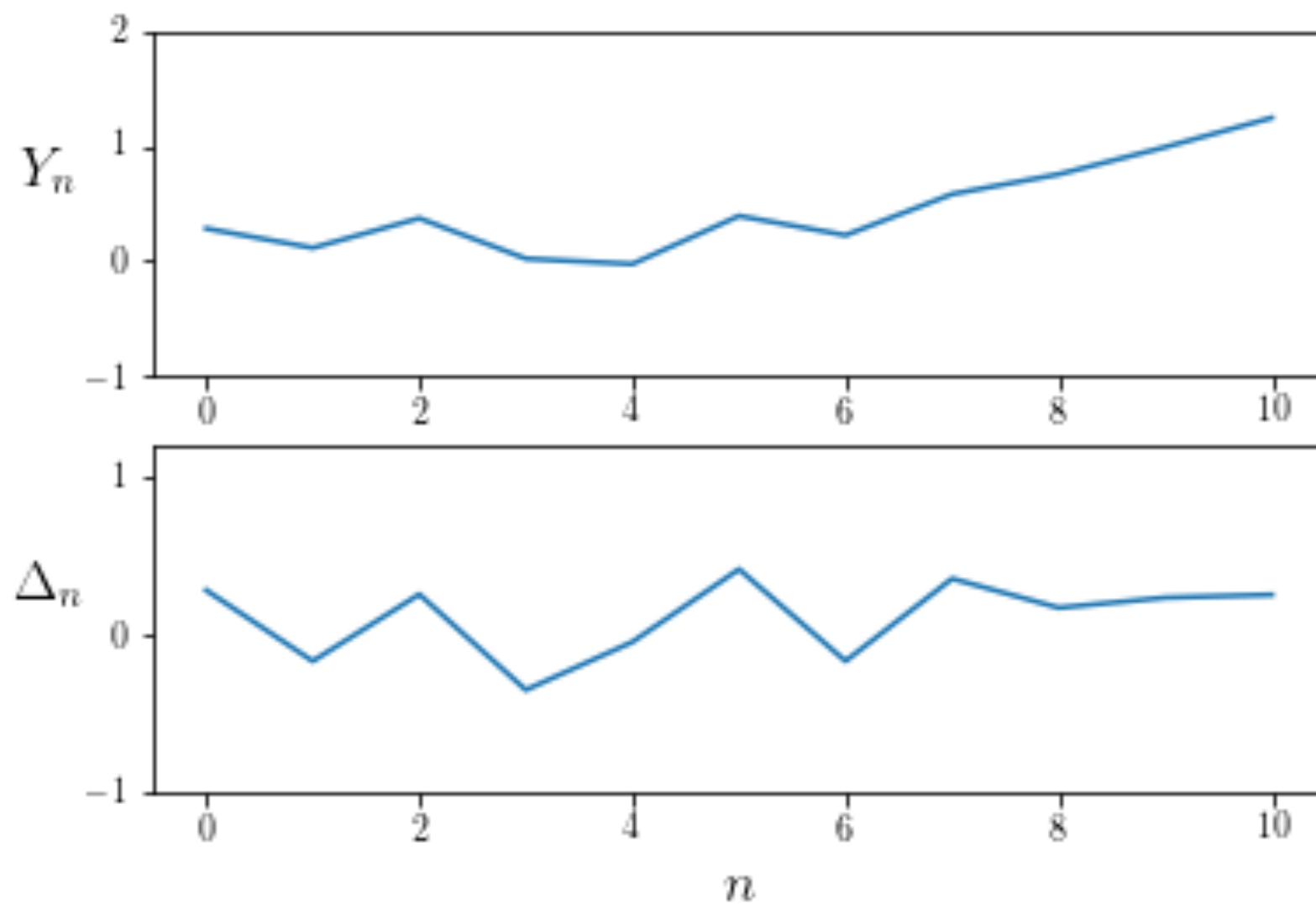
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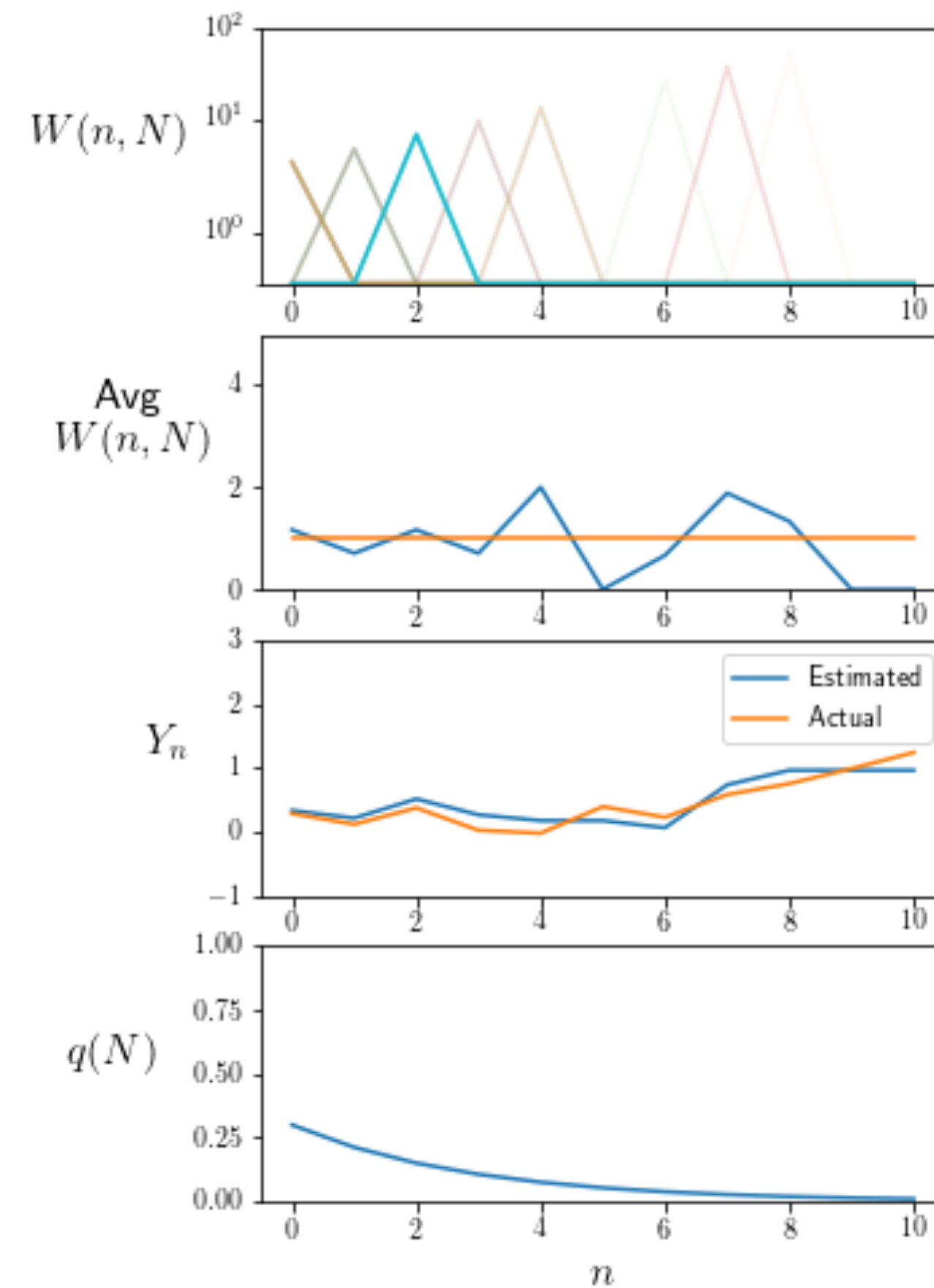
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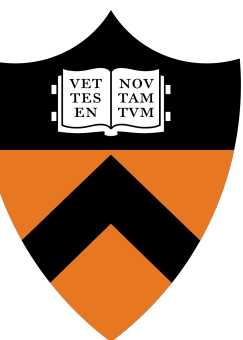
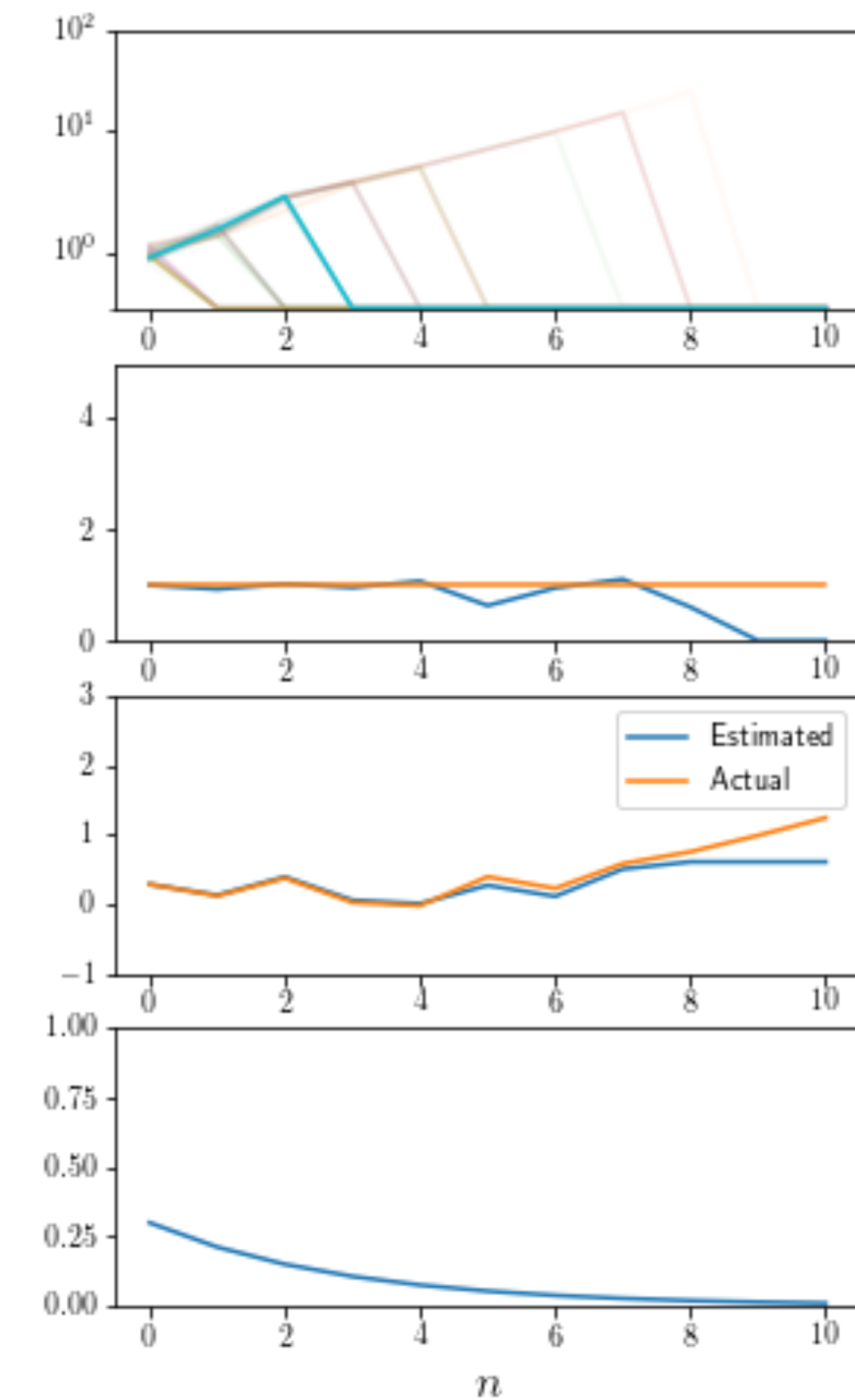
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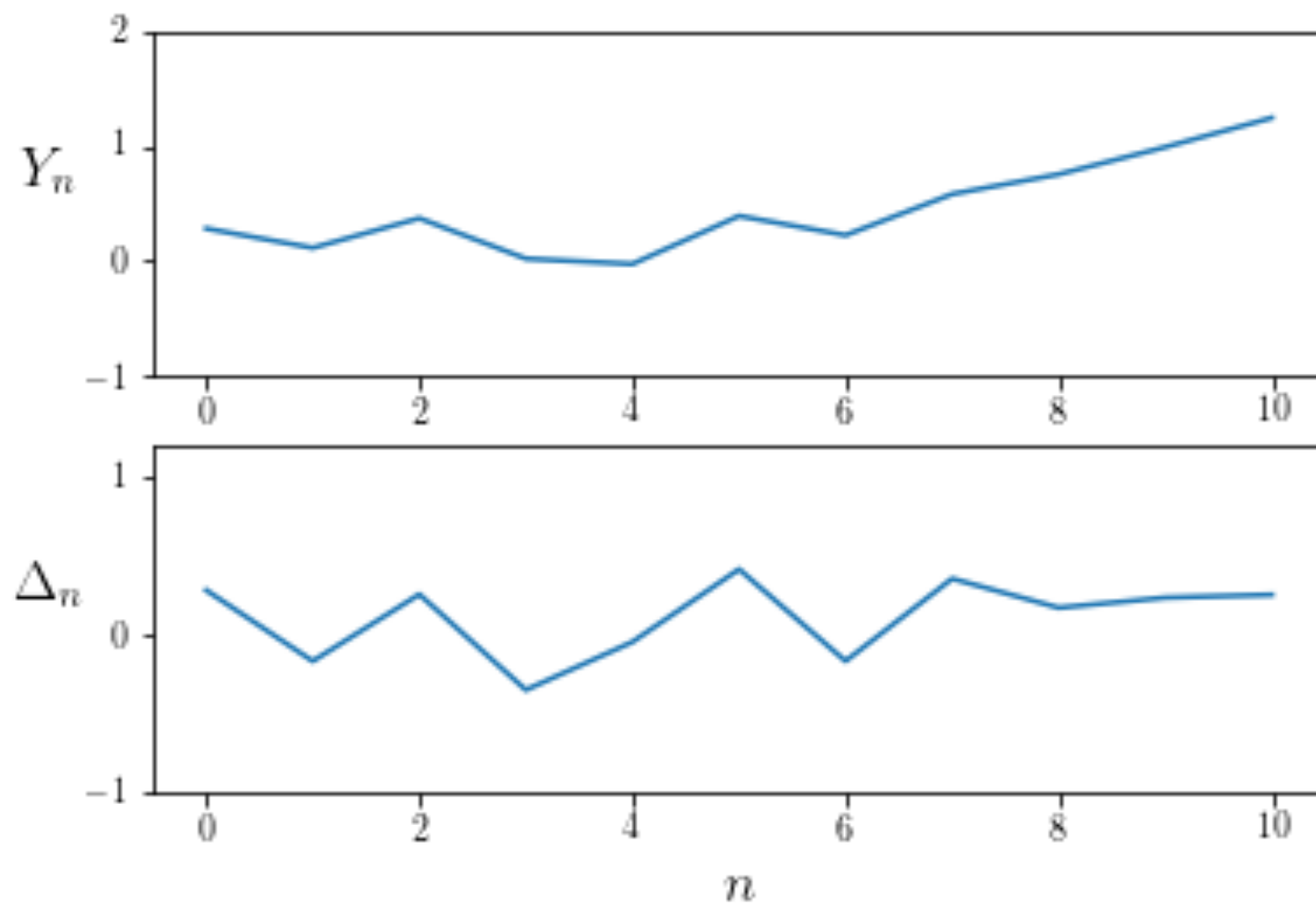
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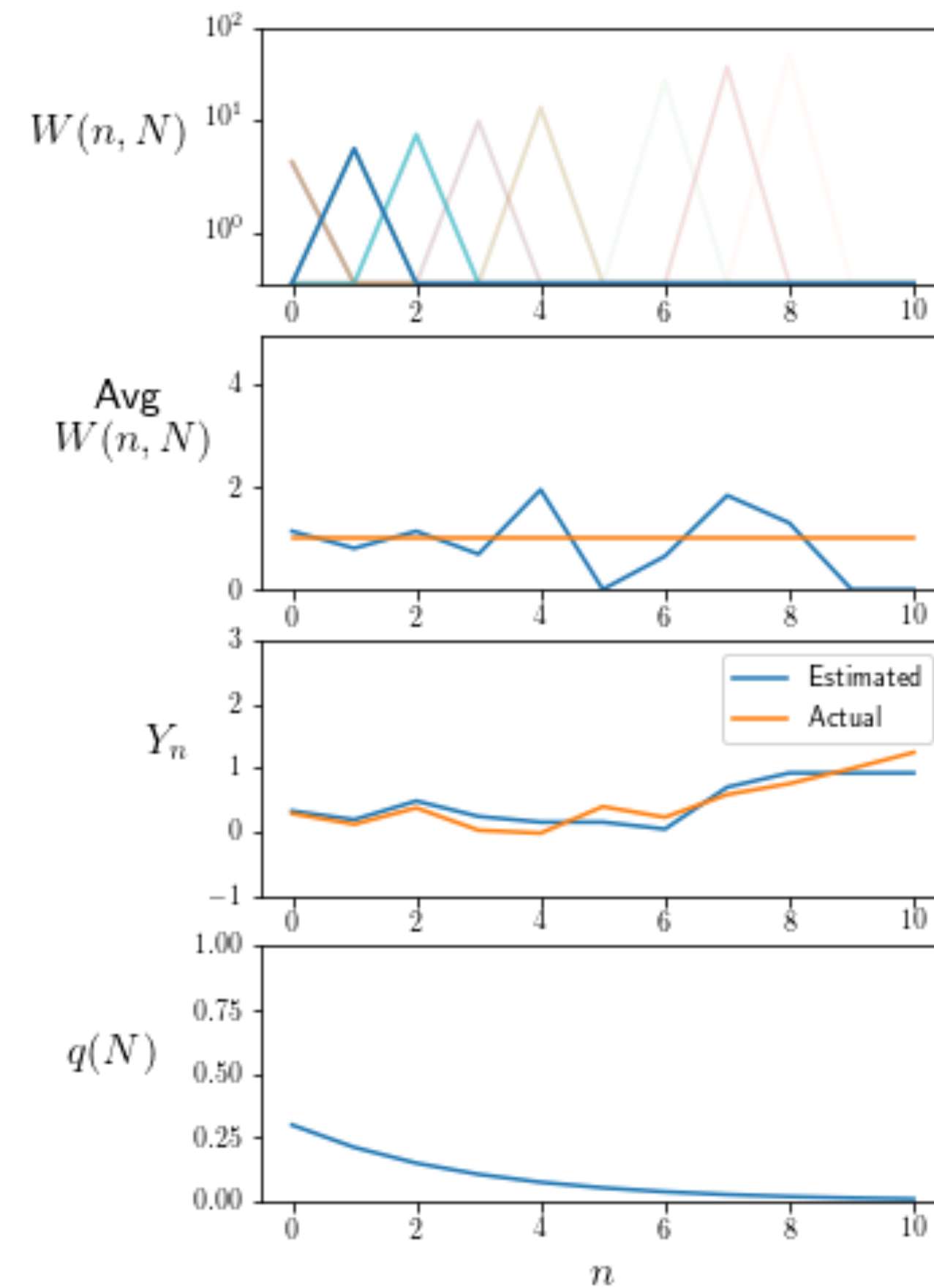
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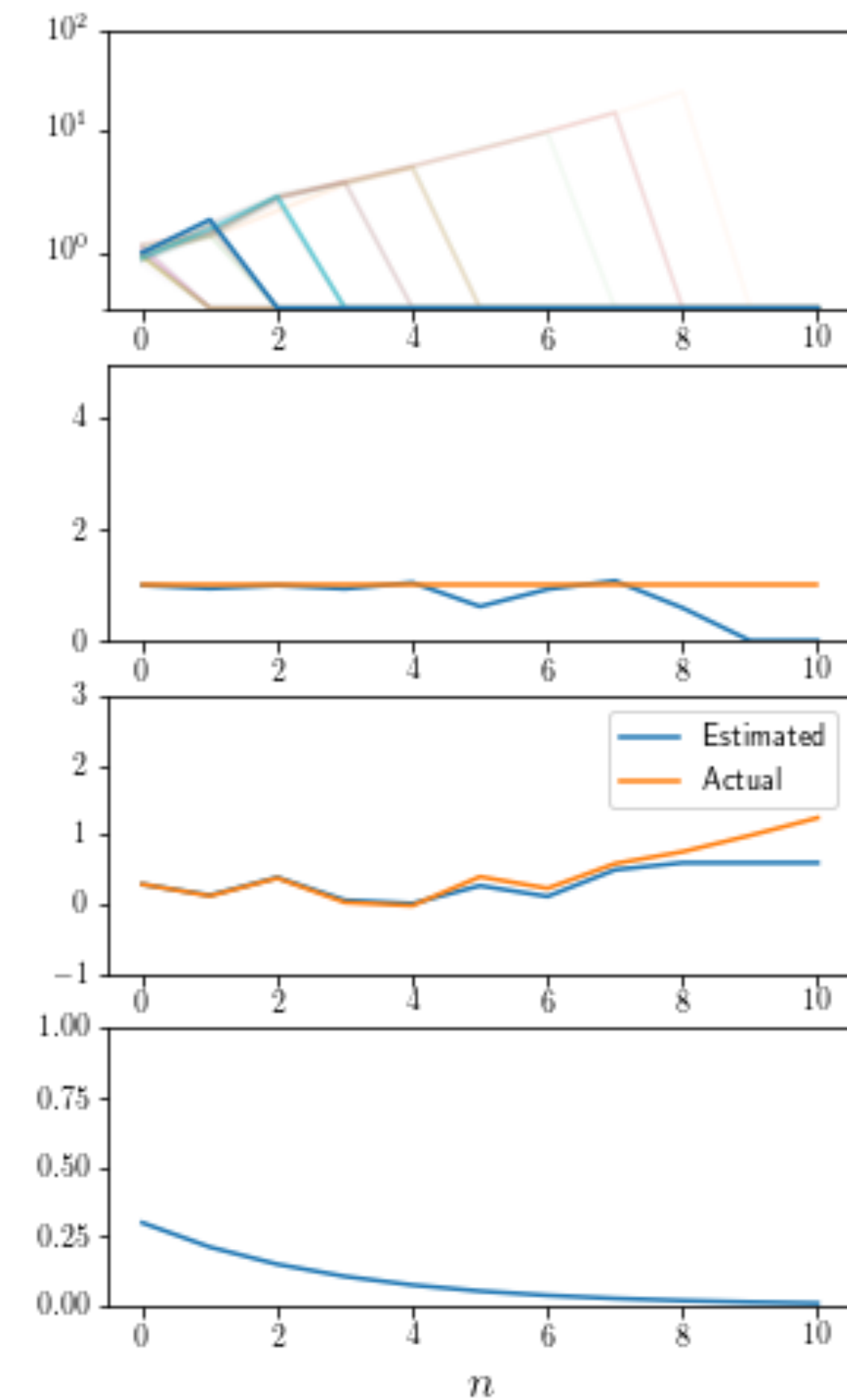
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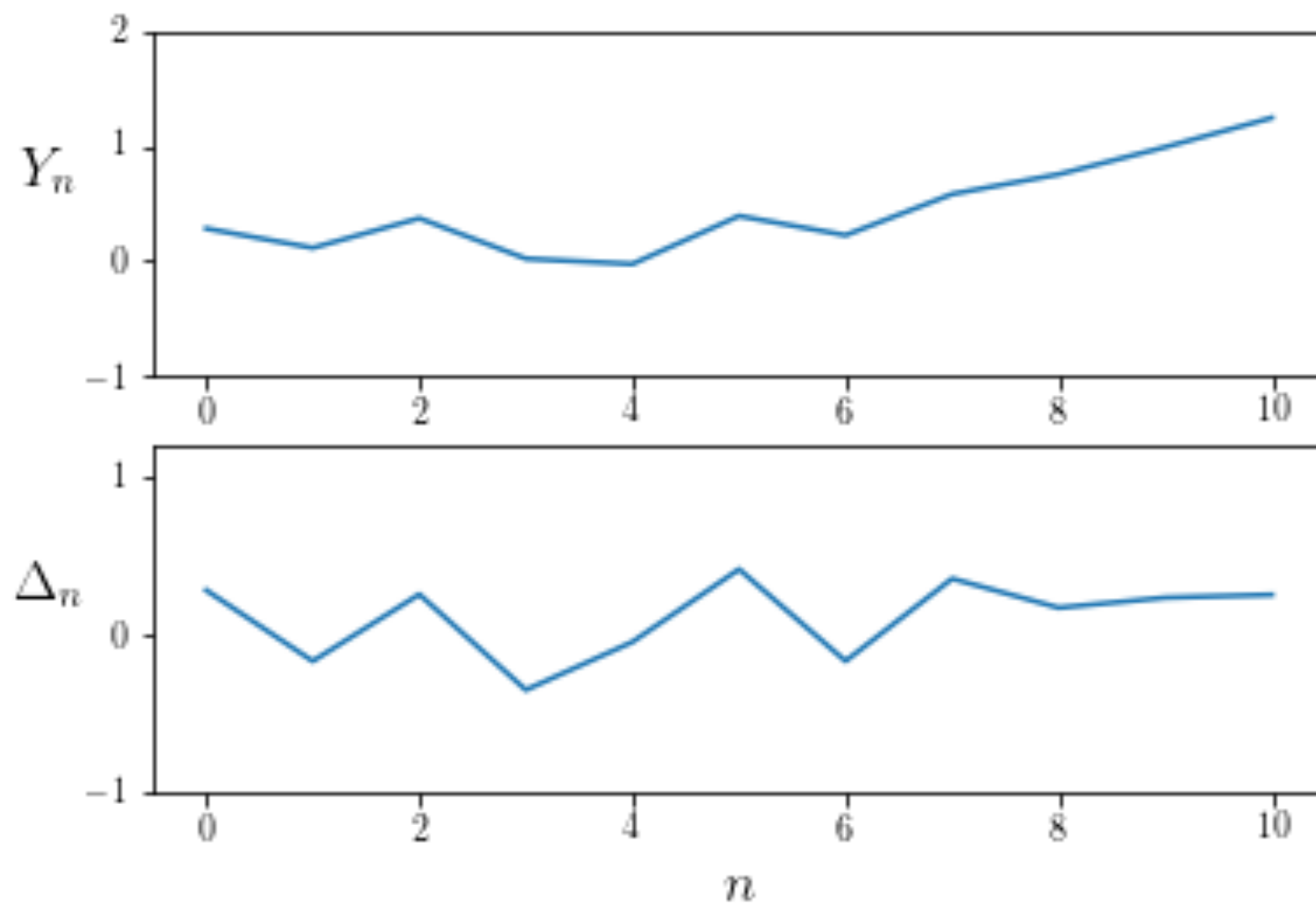
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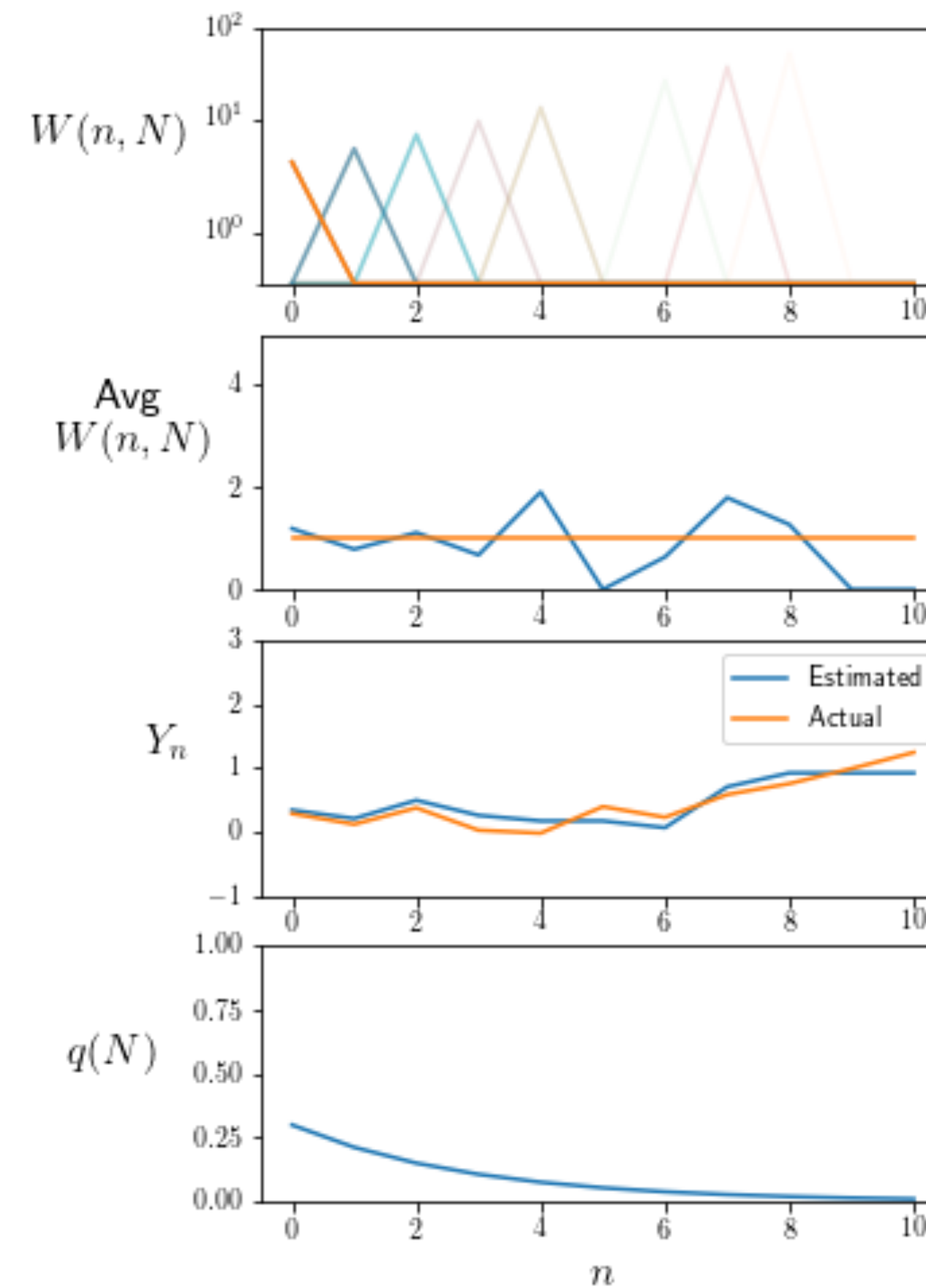
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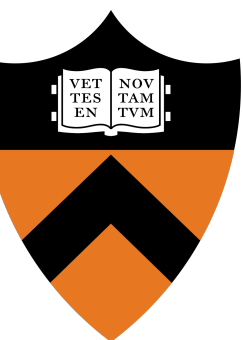
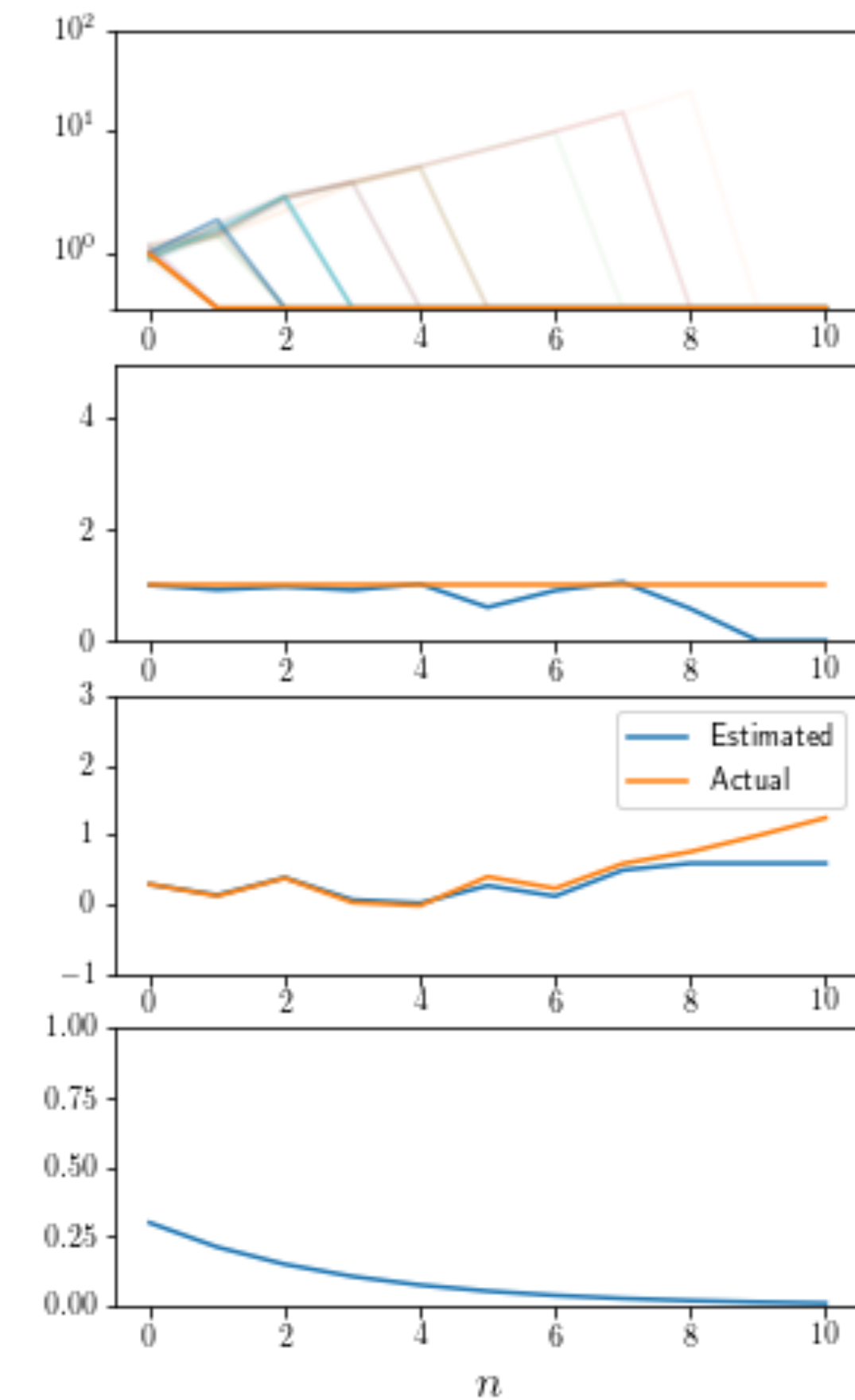
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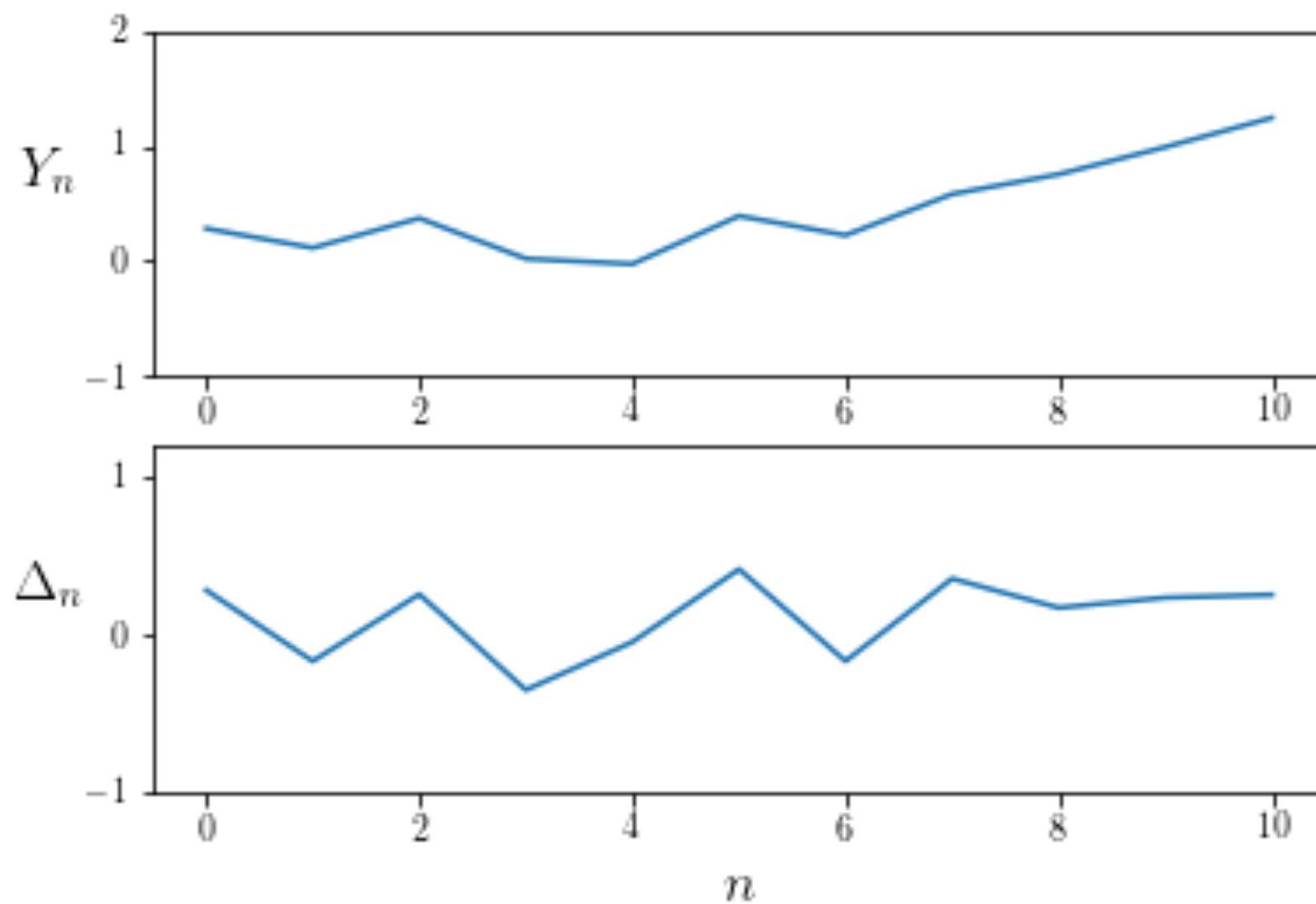
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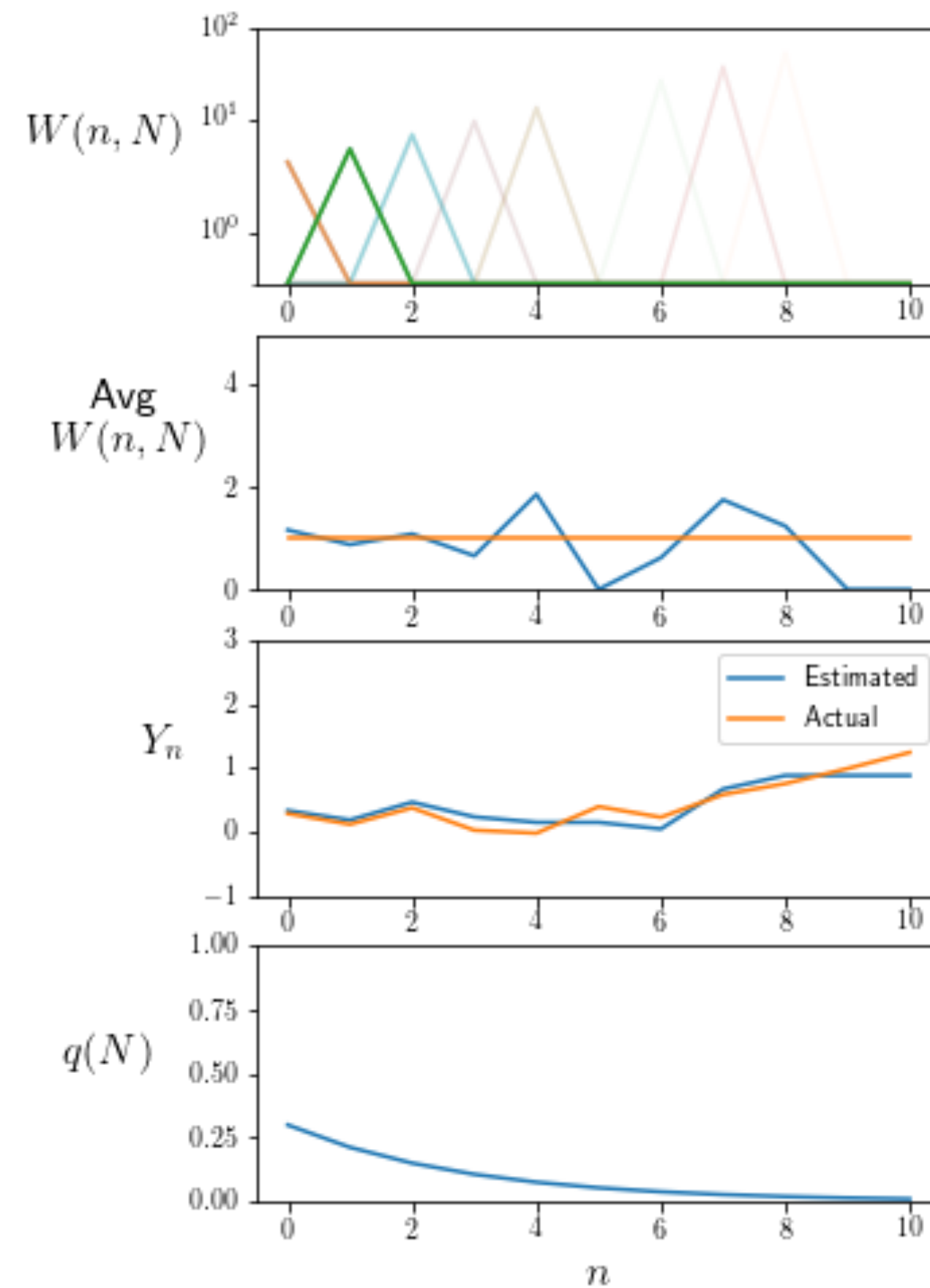
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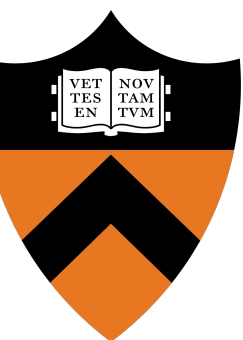
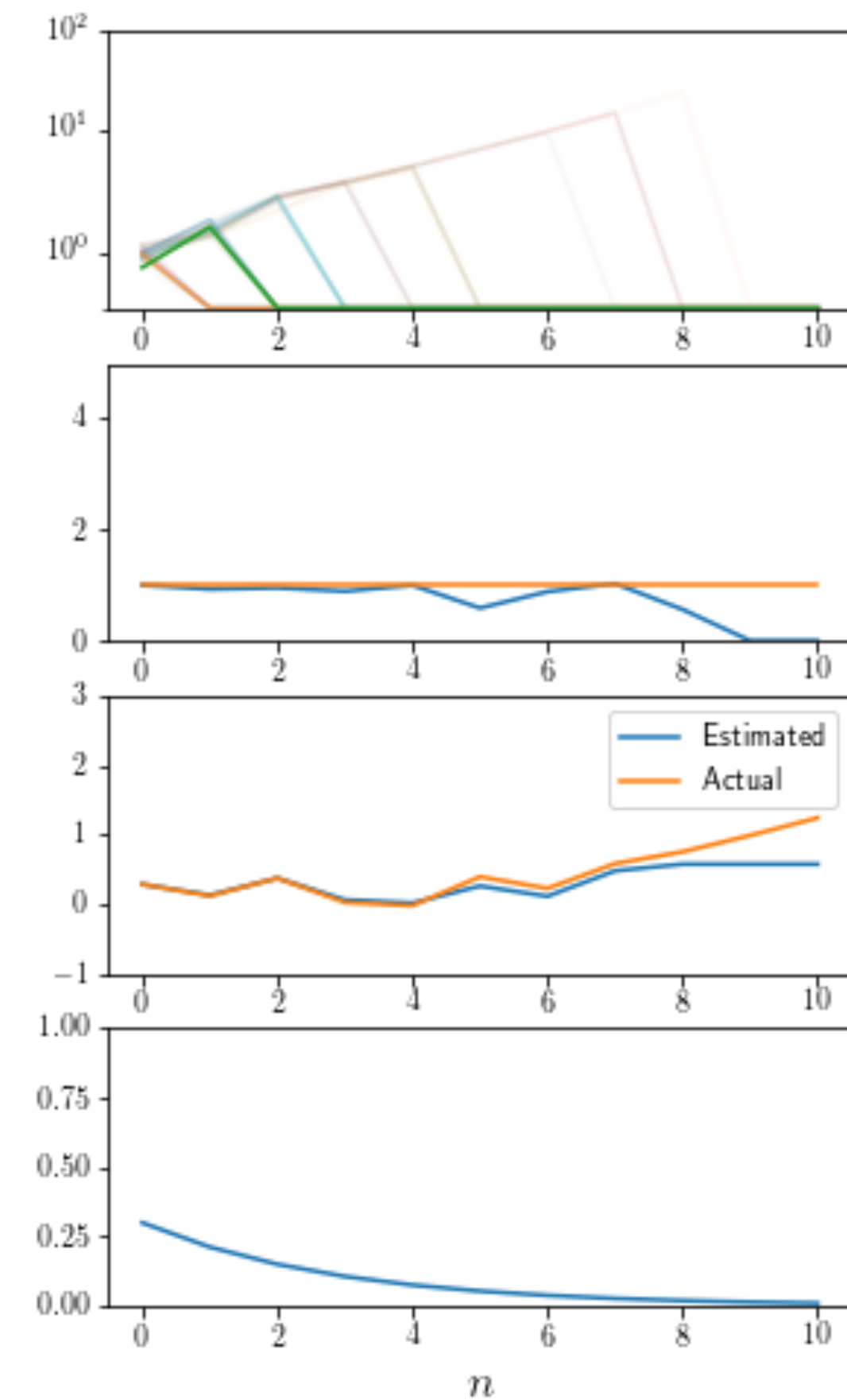
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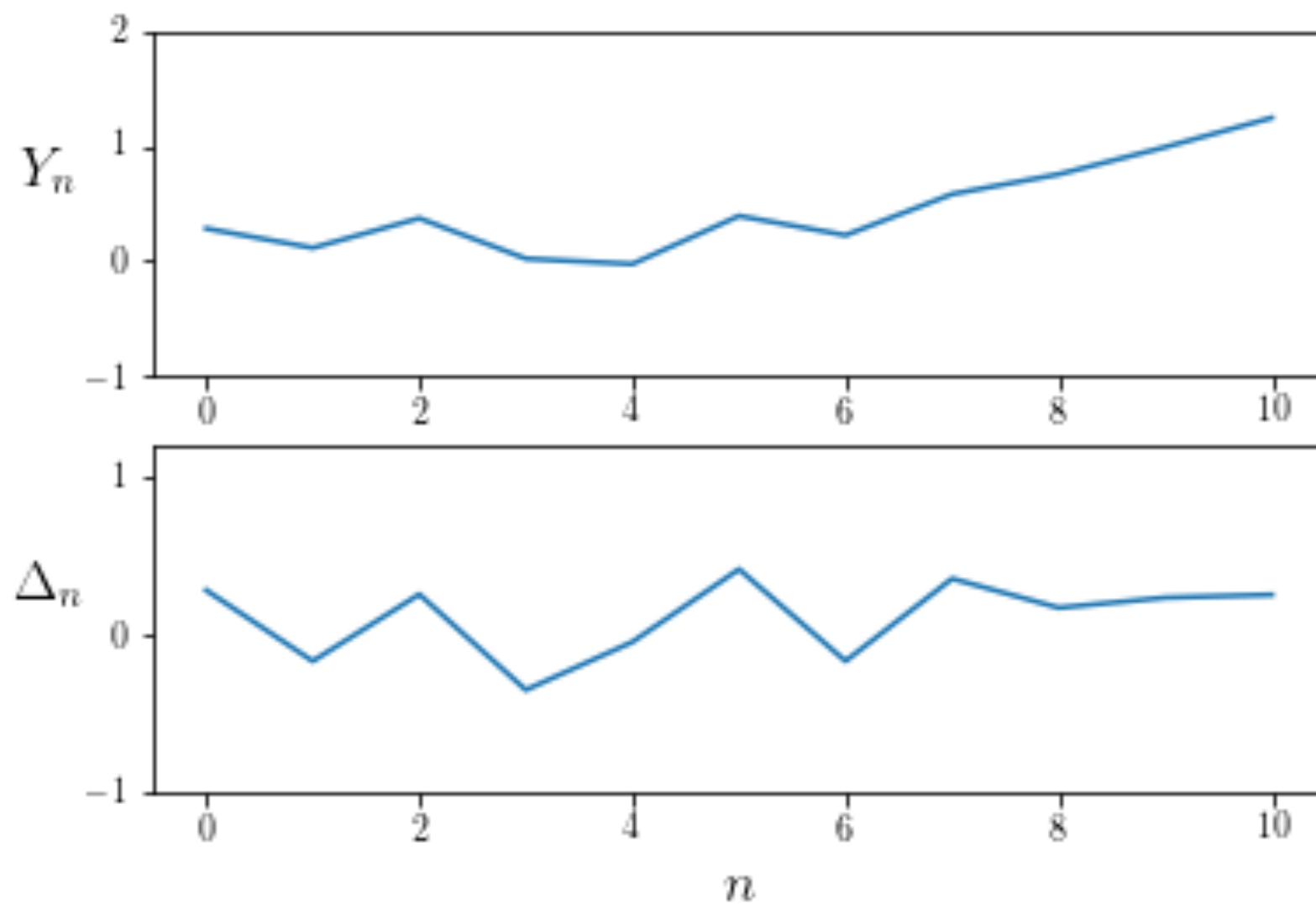
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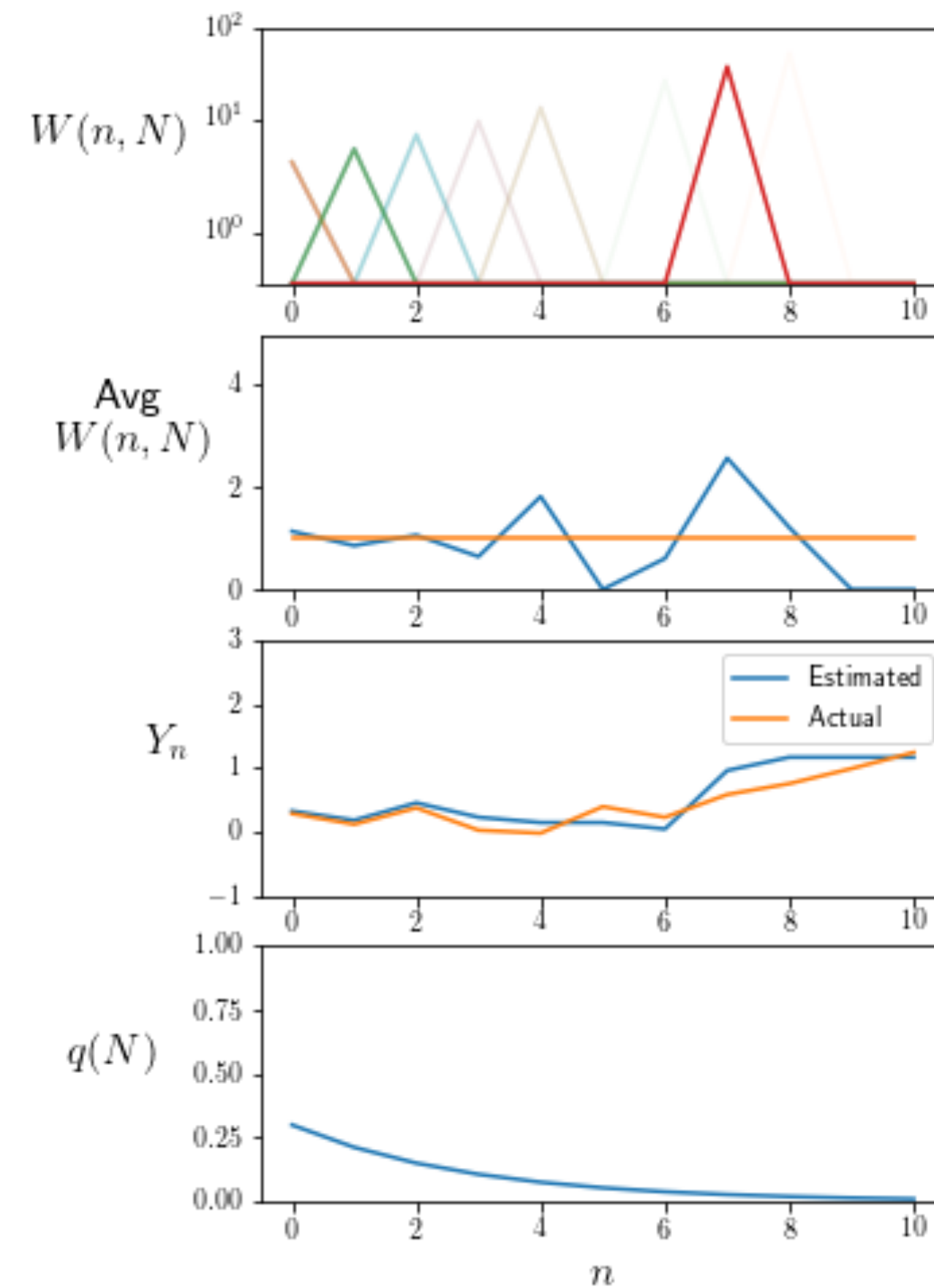
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Ground truth



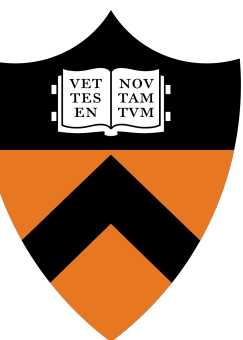
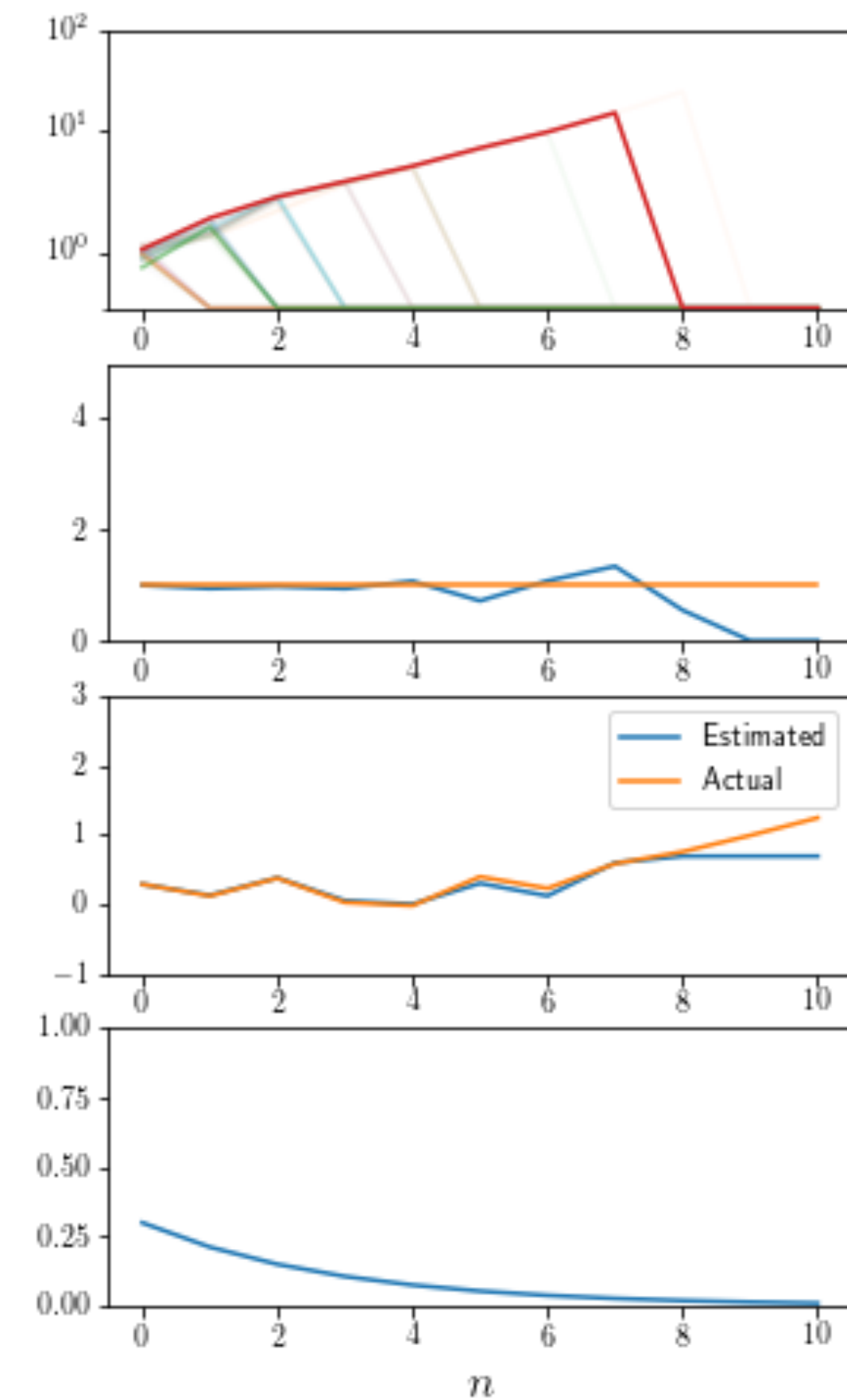
“Single sample”

$$W(n, N) = \frac{1}{q(N)} \mathbb{1}\{n = N\}$$



“Russian roulette”

$$W(n, N) = \frac{1}{1 - \sum_{n'=1}^{n-1} q(n')} \mathbb{1}\{N \geq n\}$$



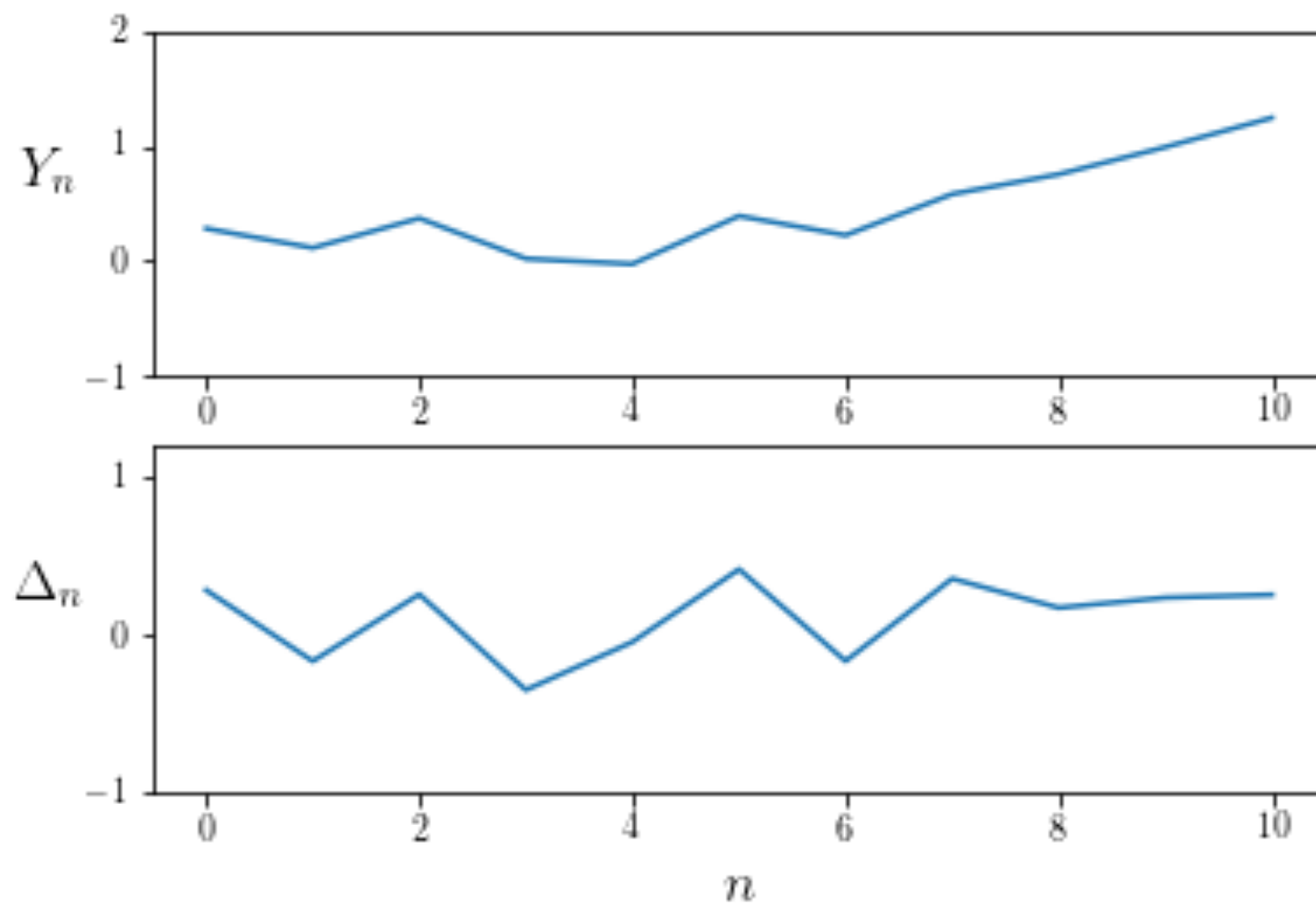
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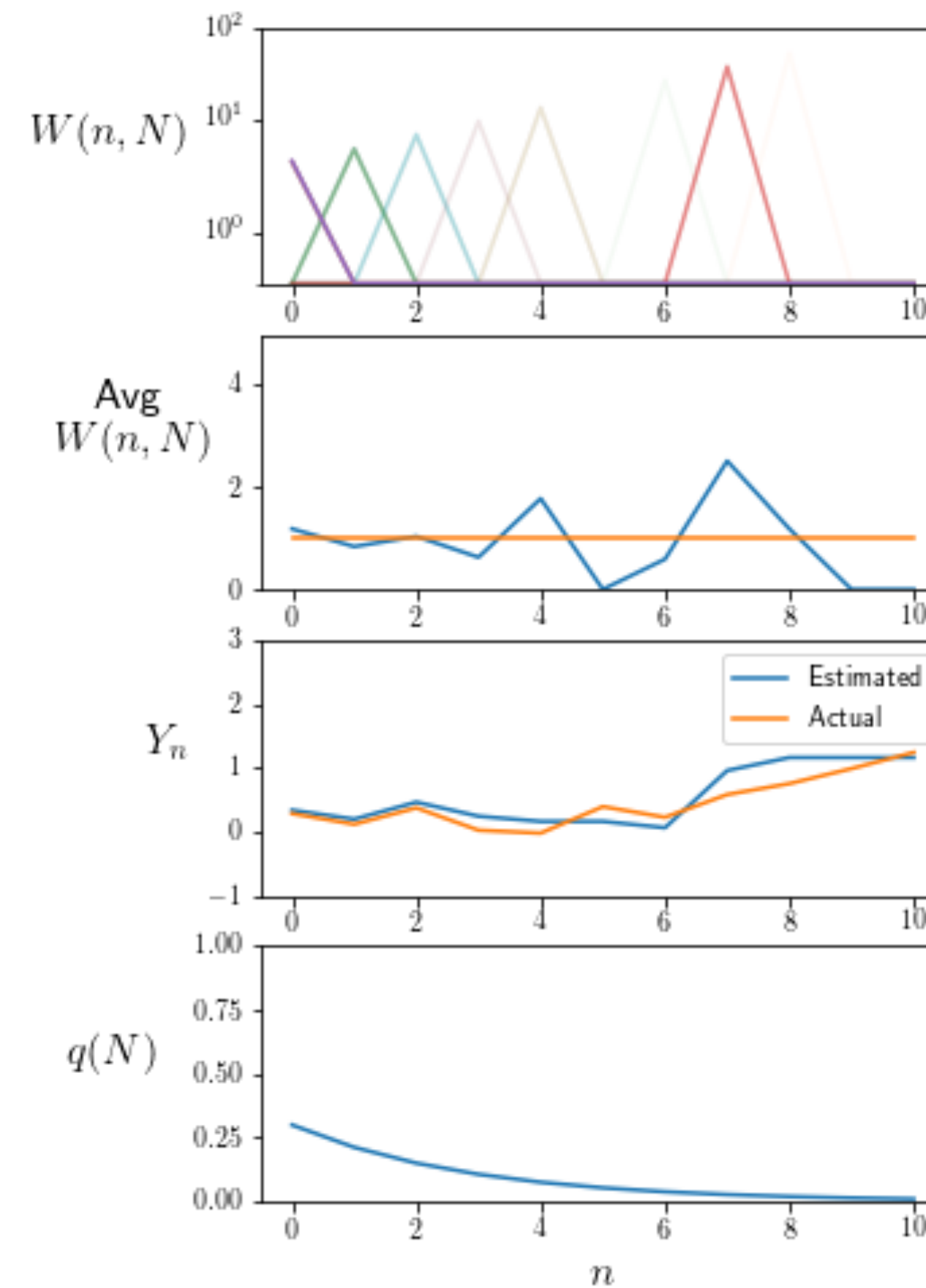
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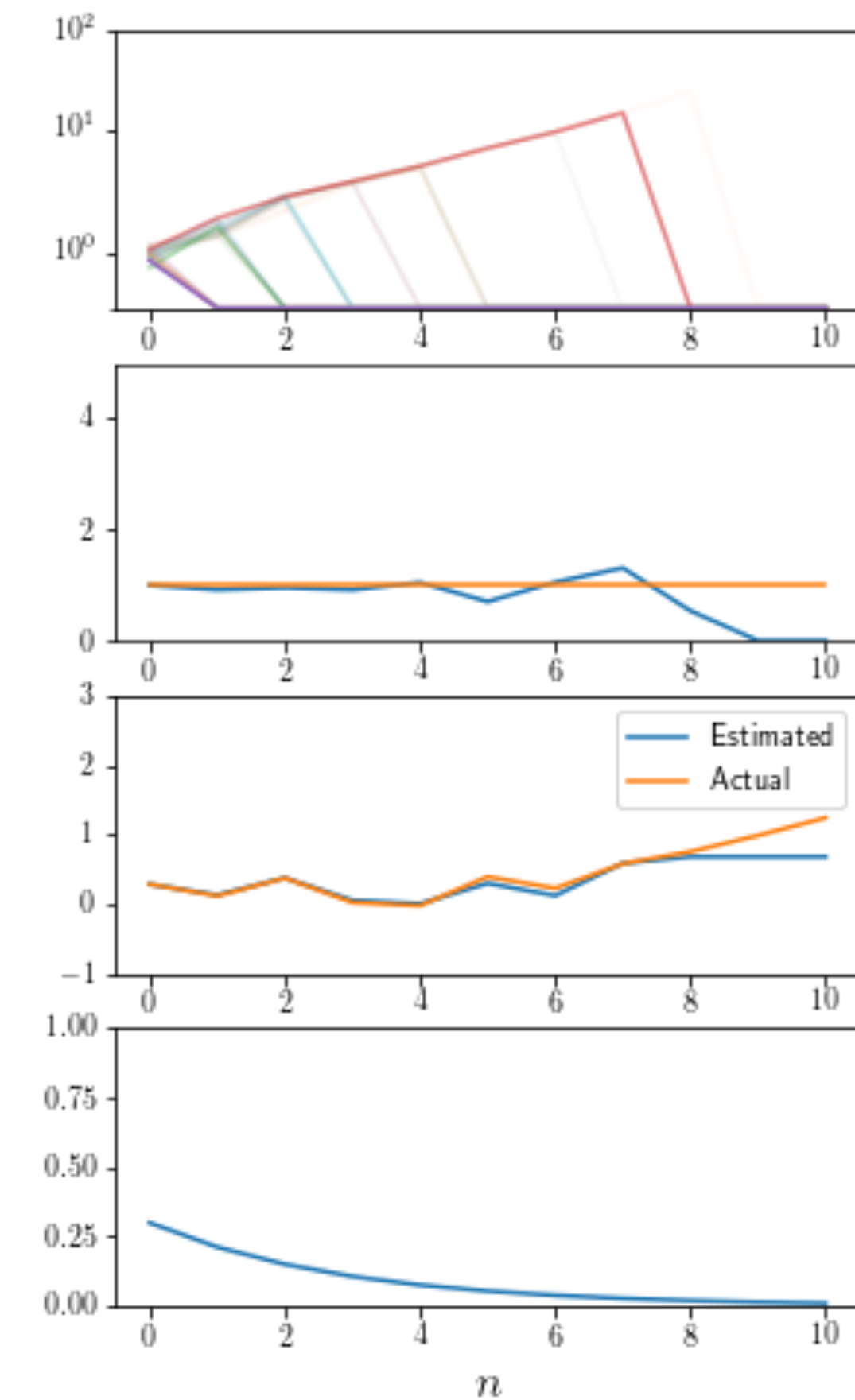
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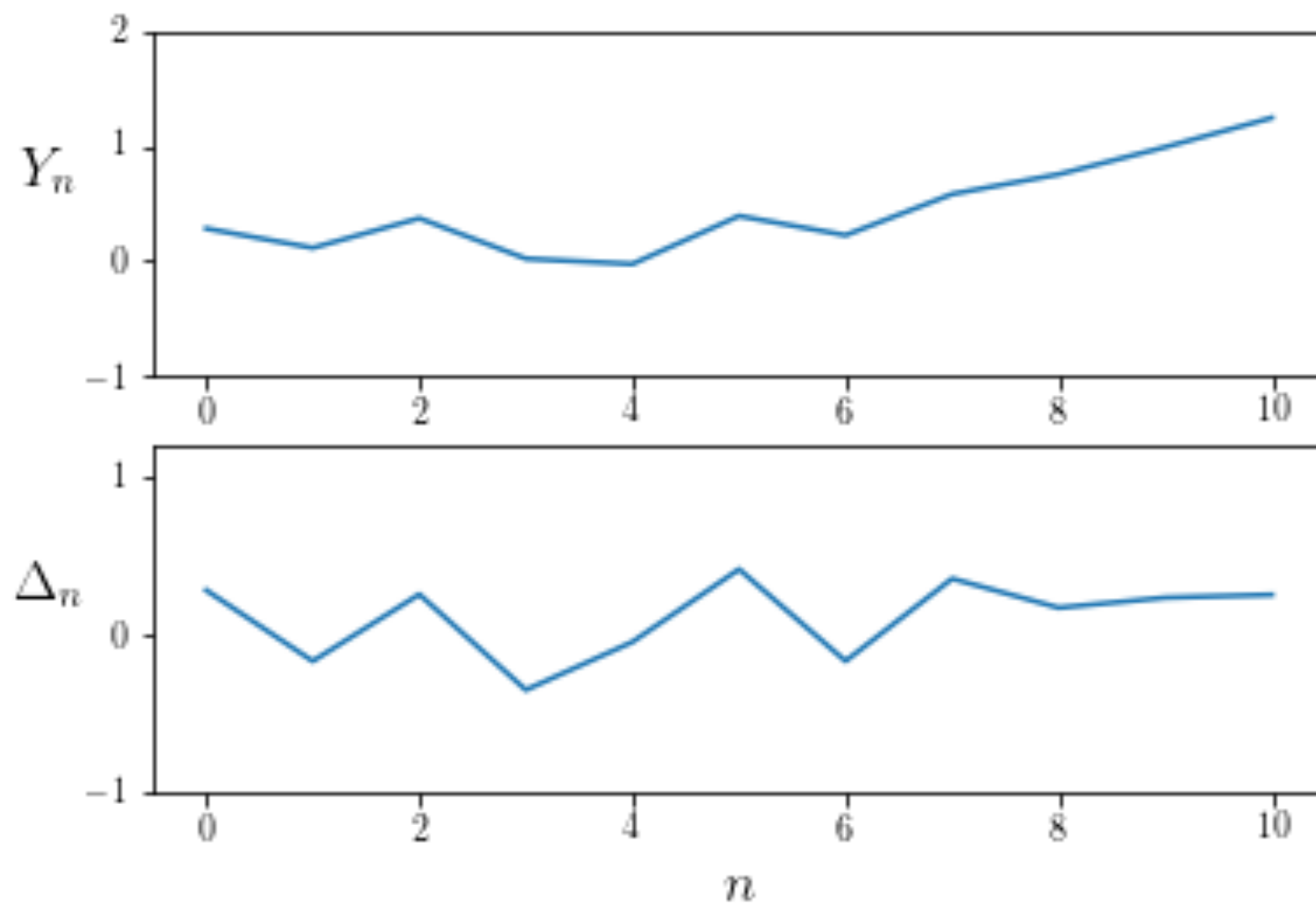
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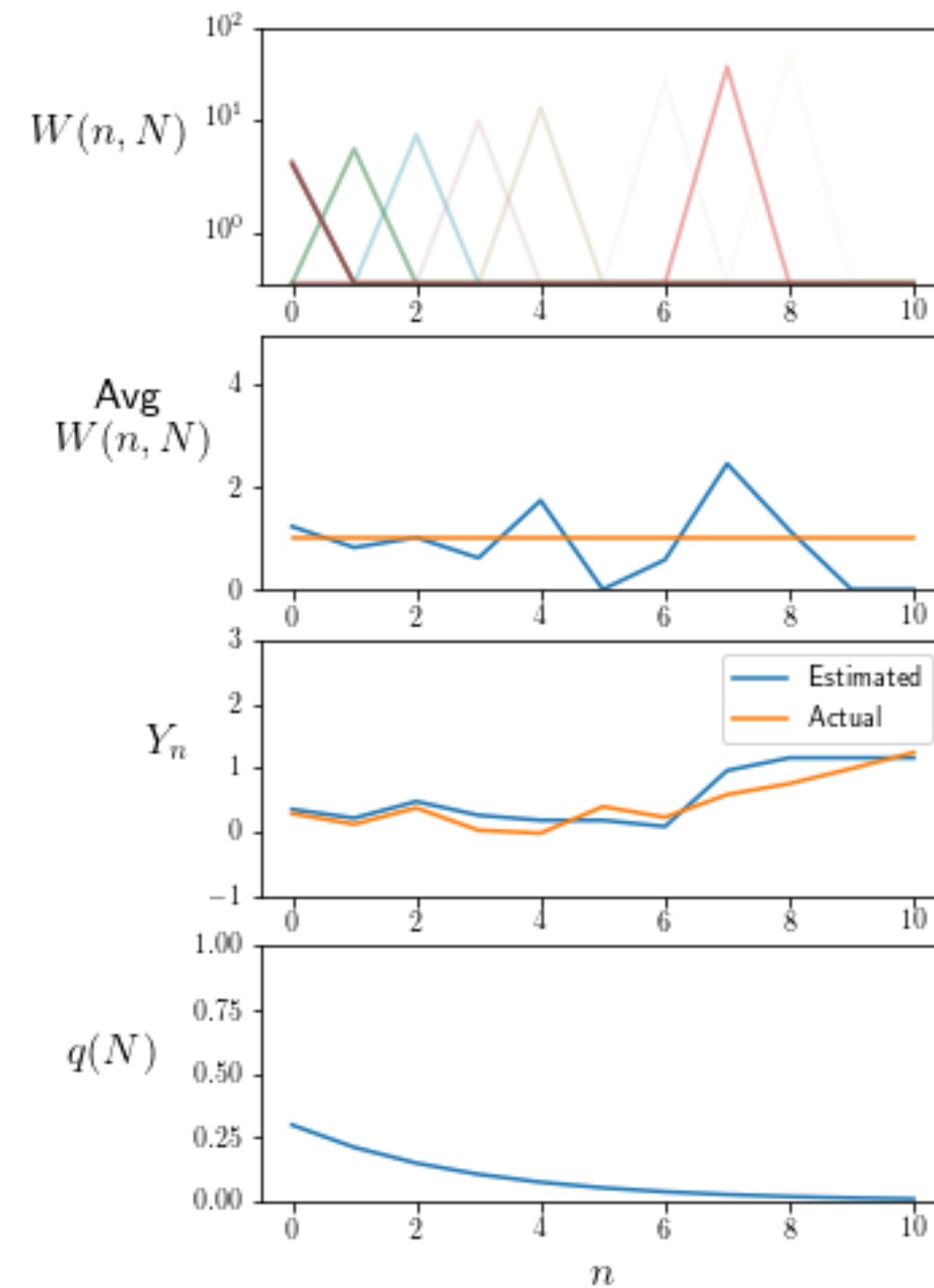
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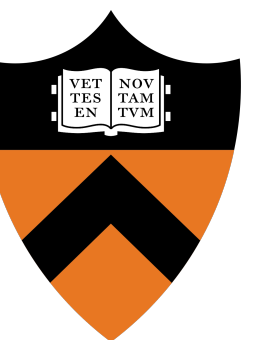
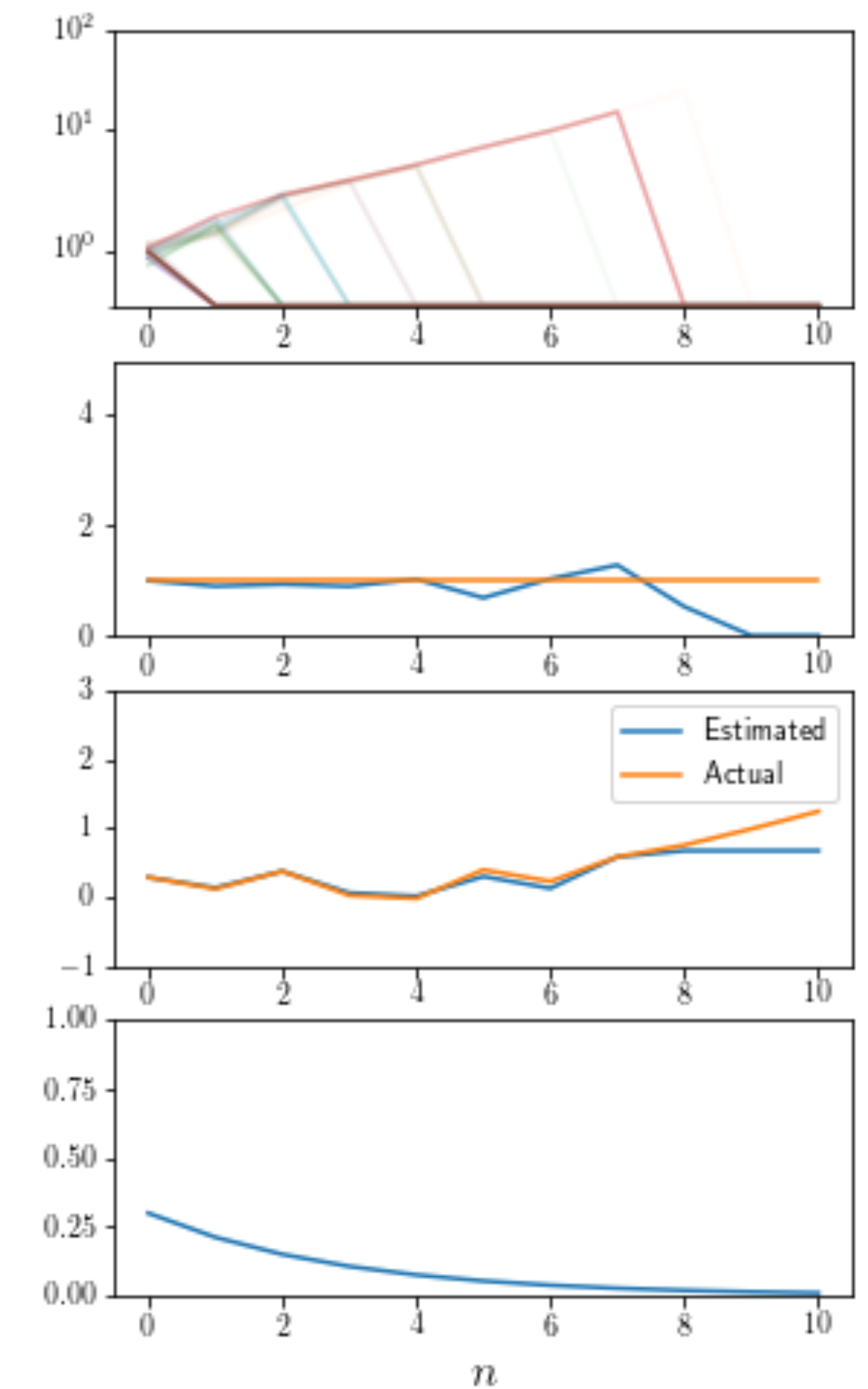
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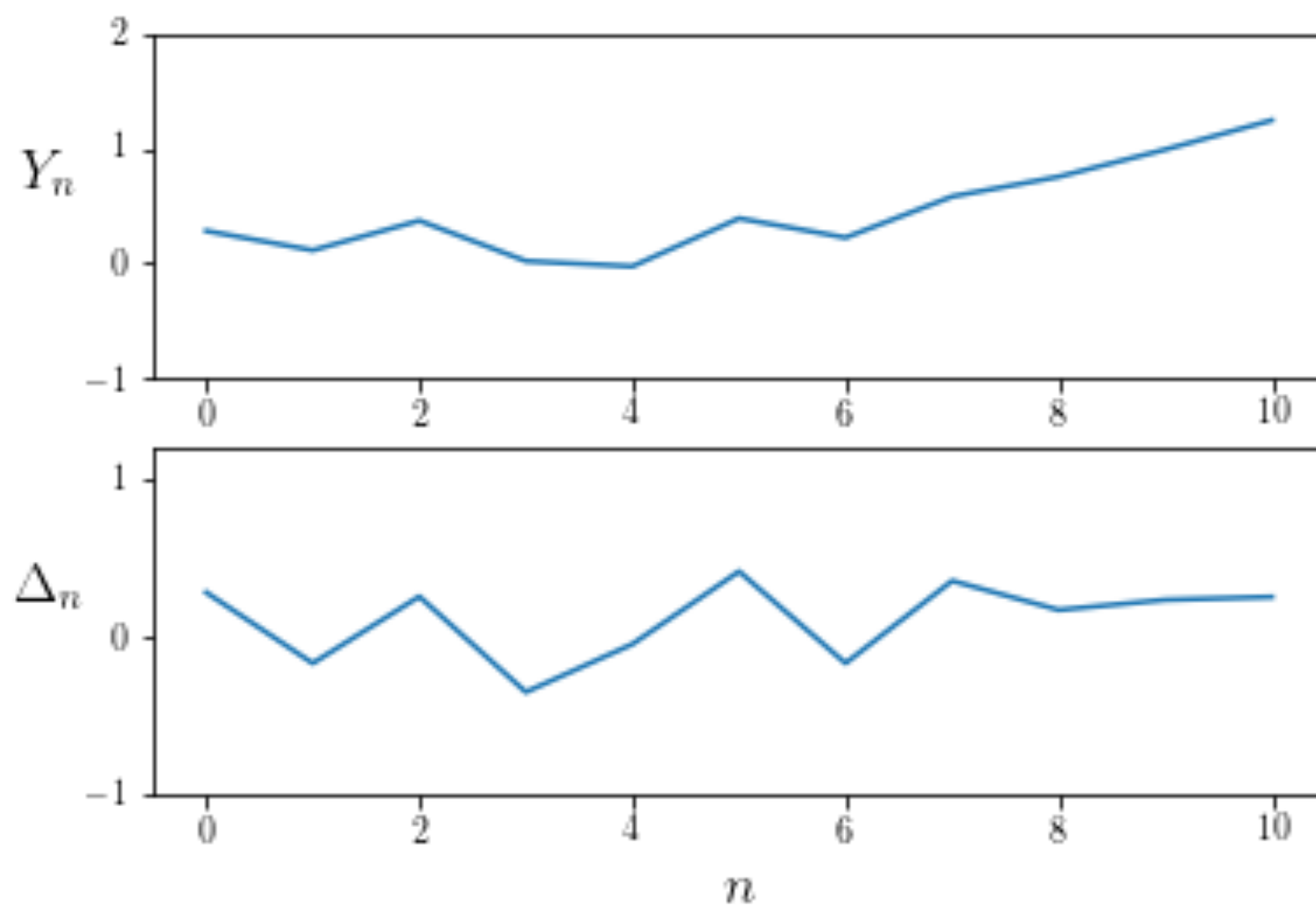
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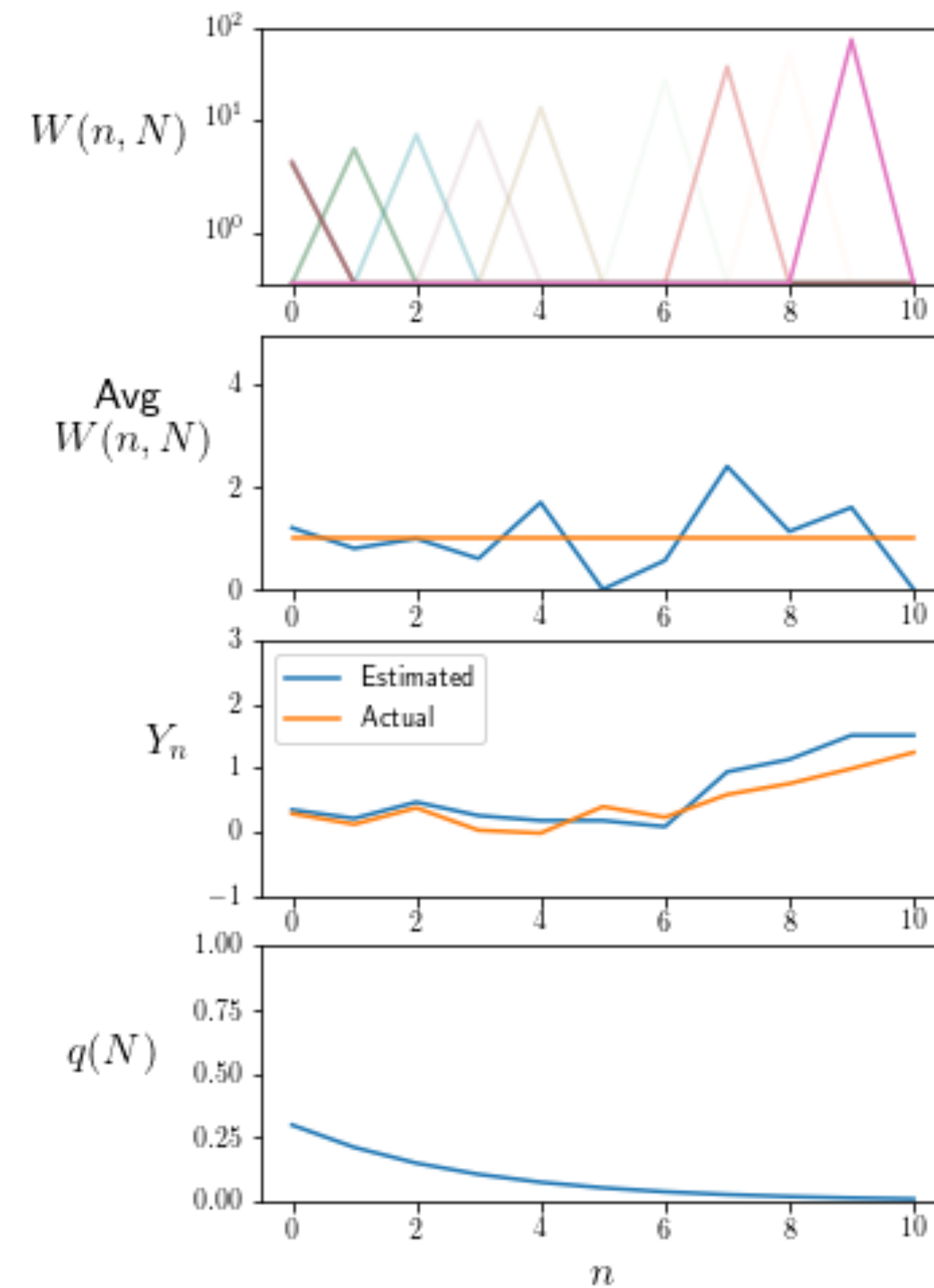
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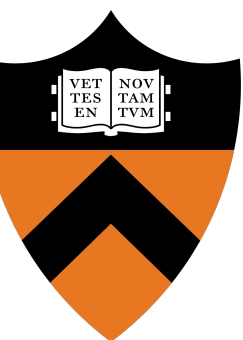
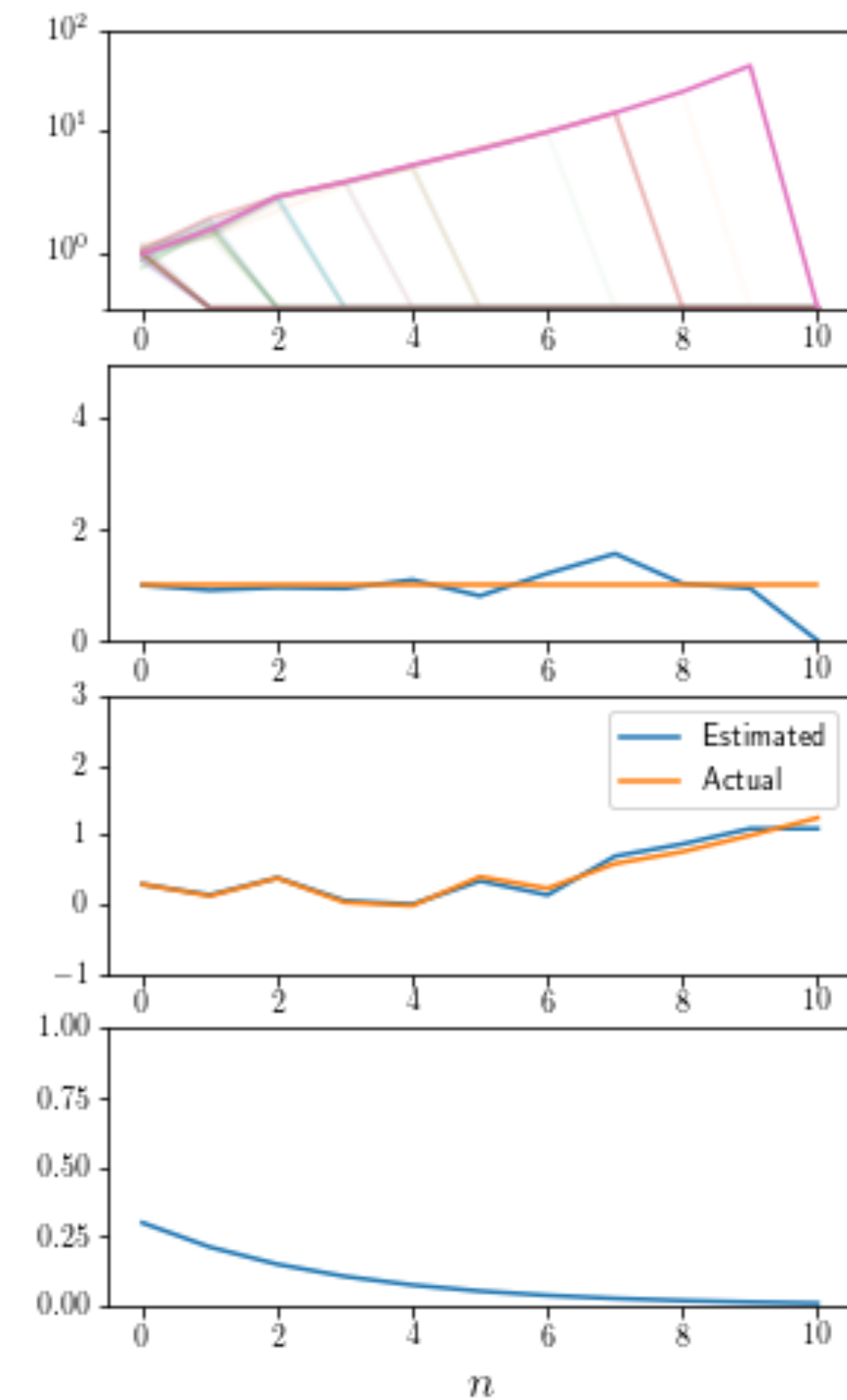
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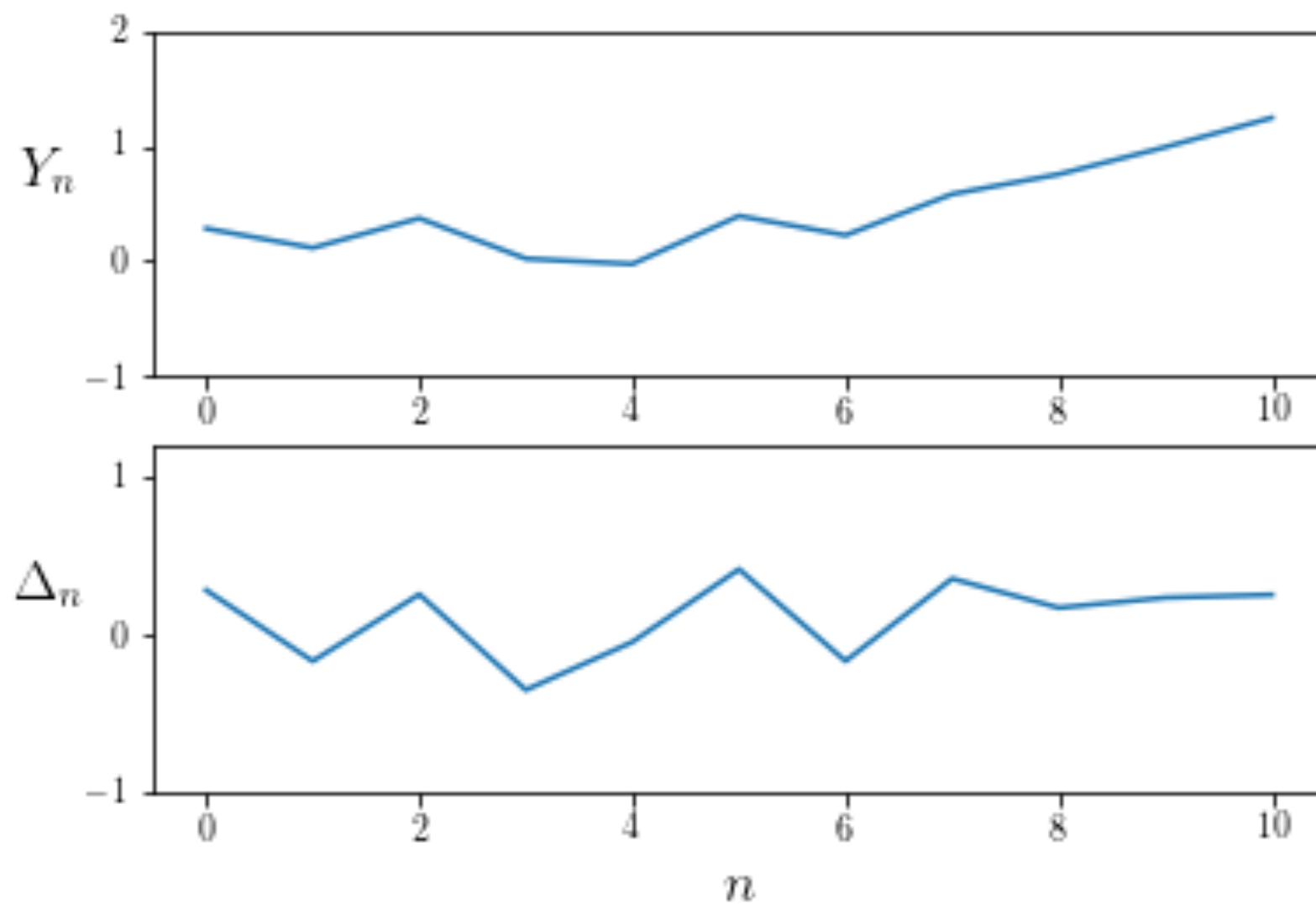
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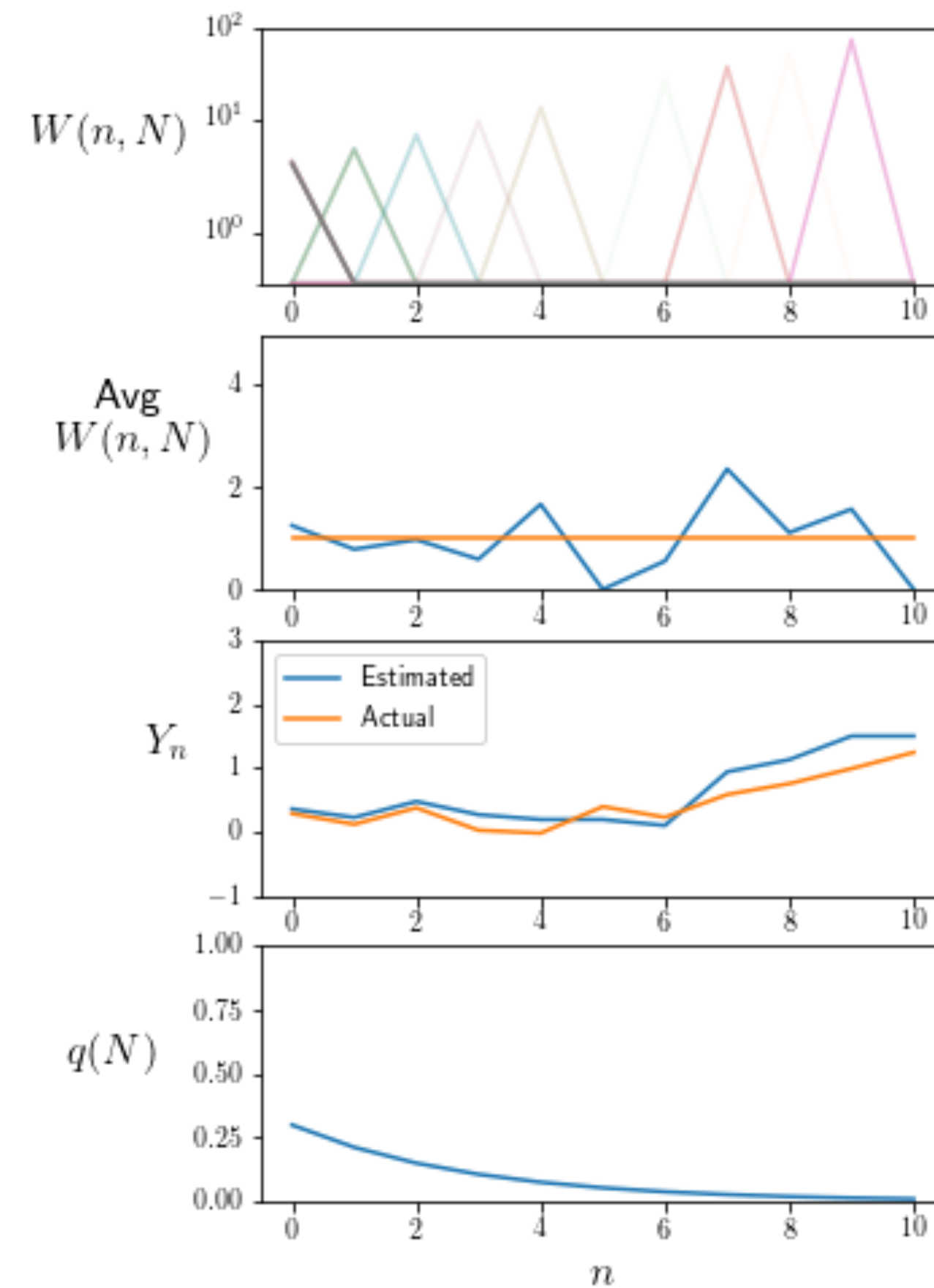
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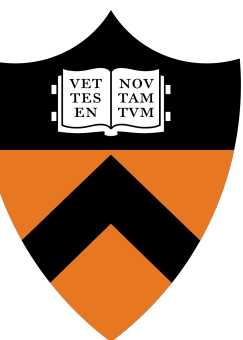
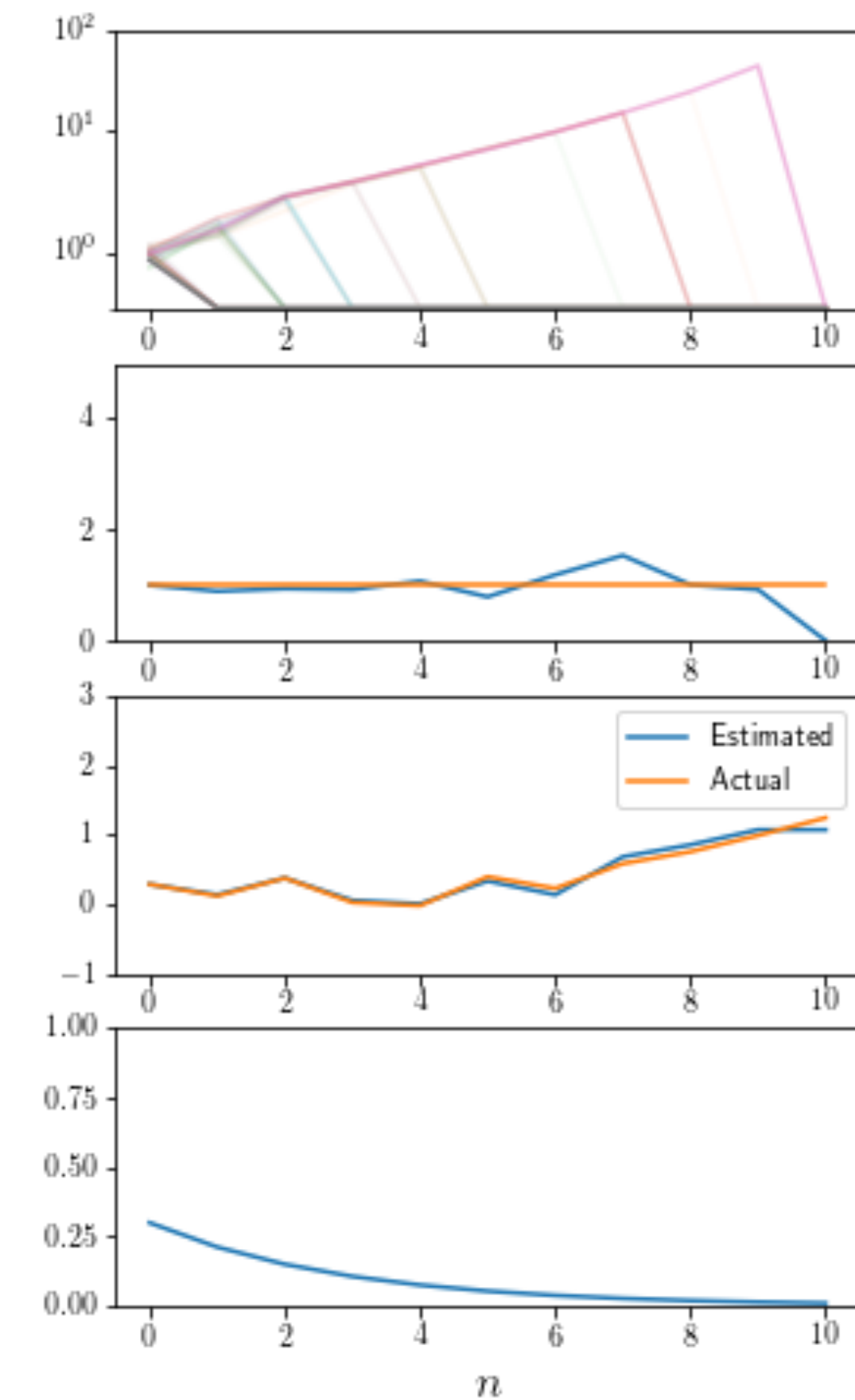
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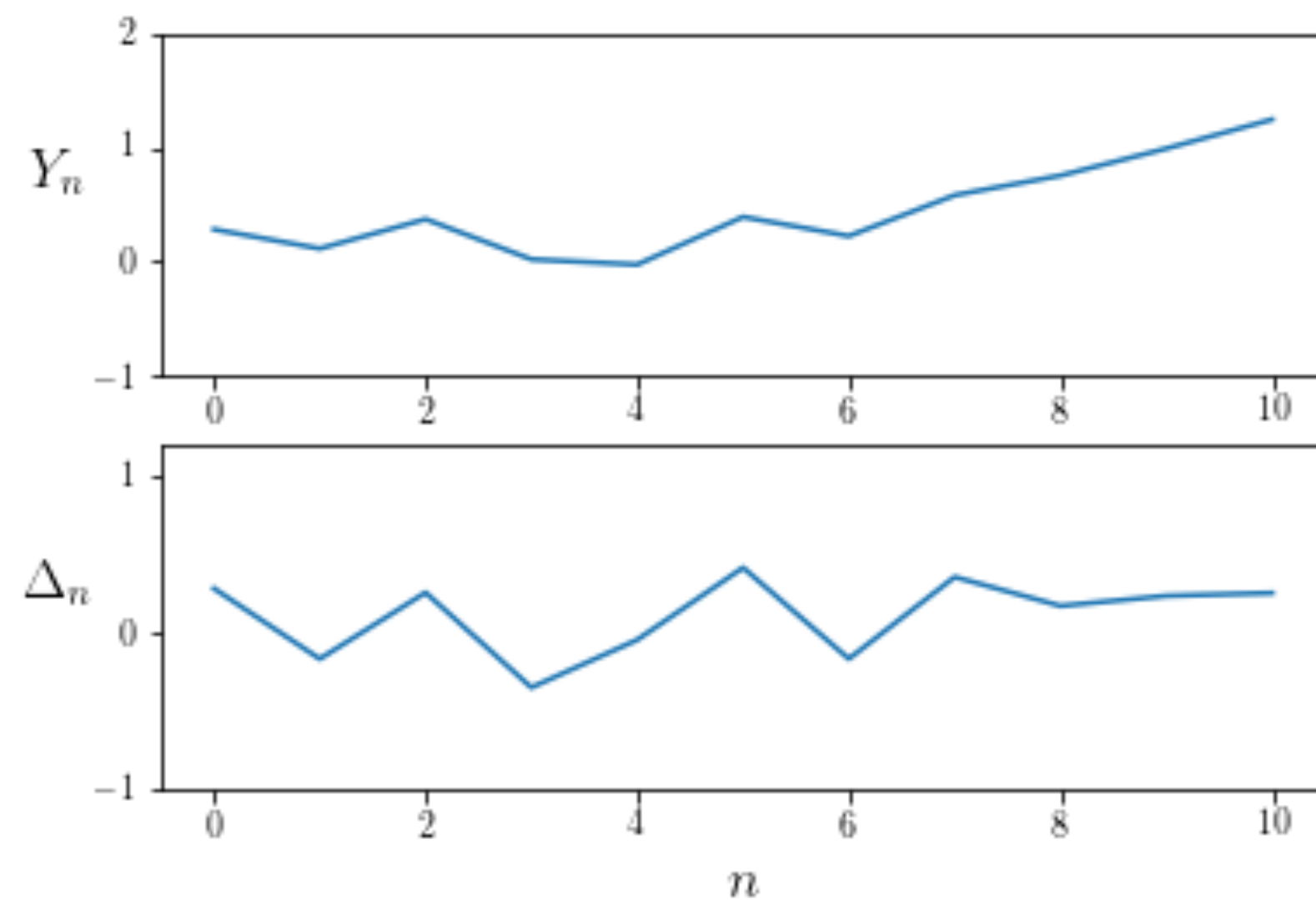
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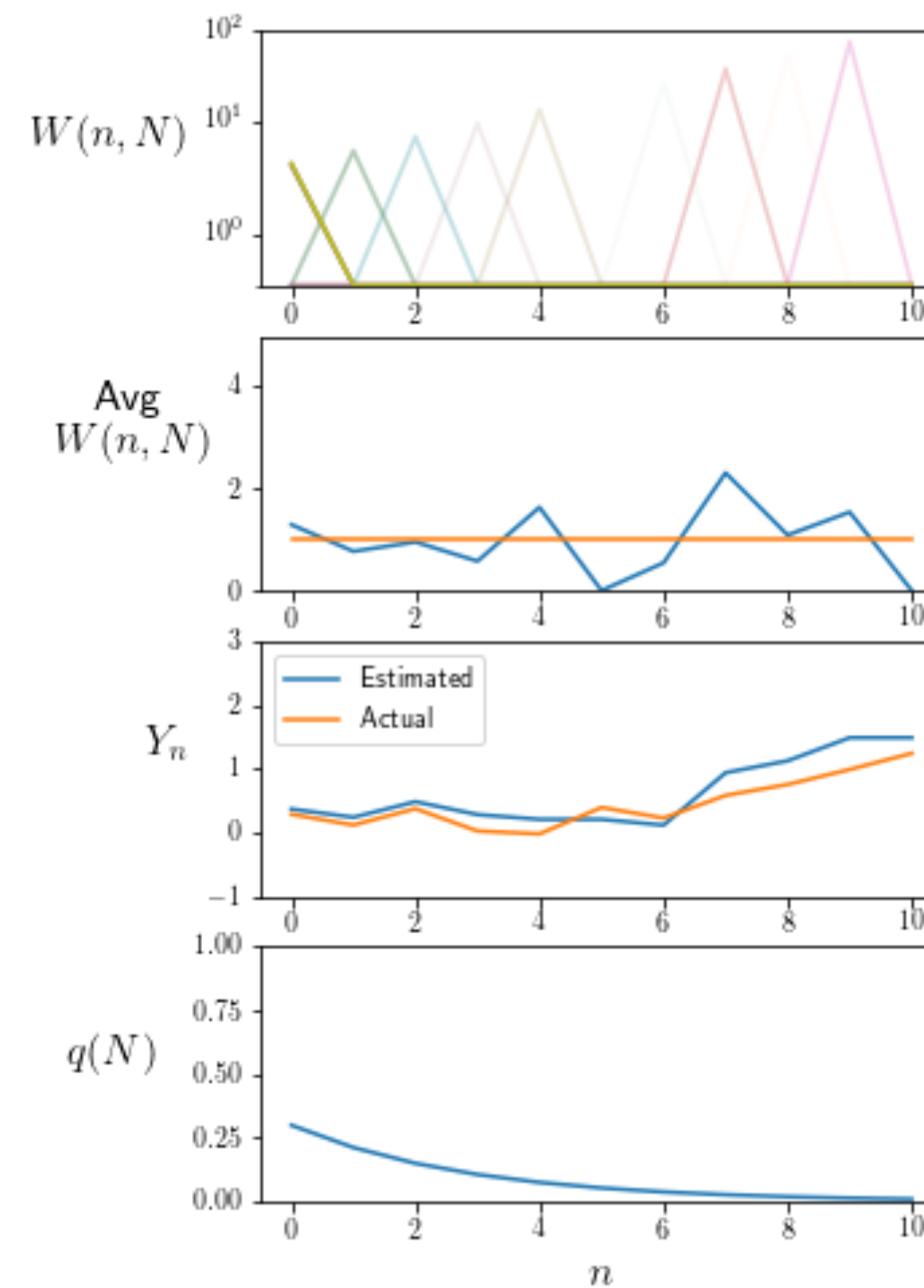
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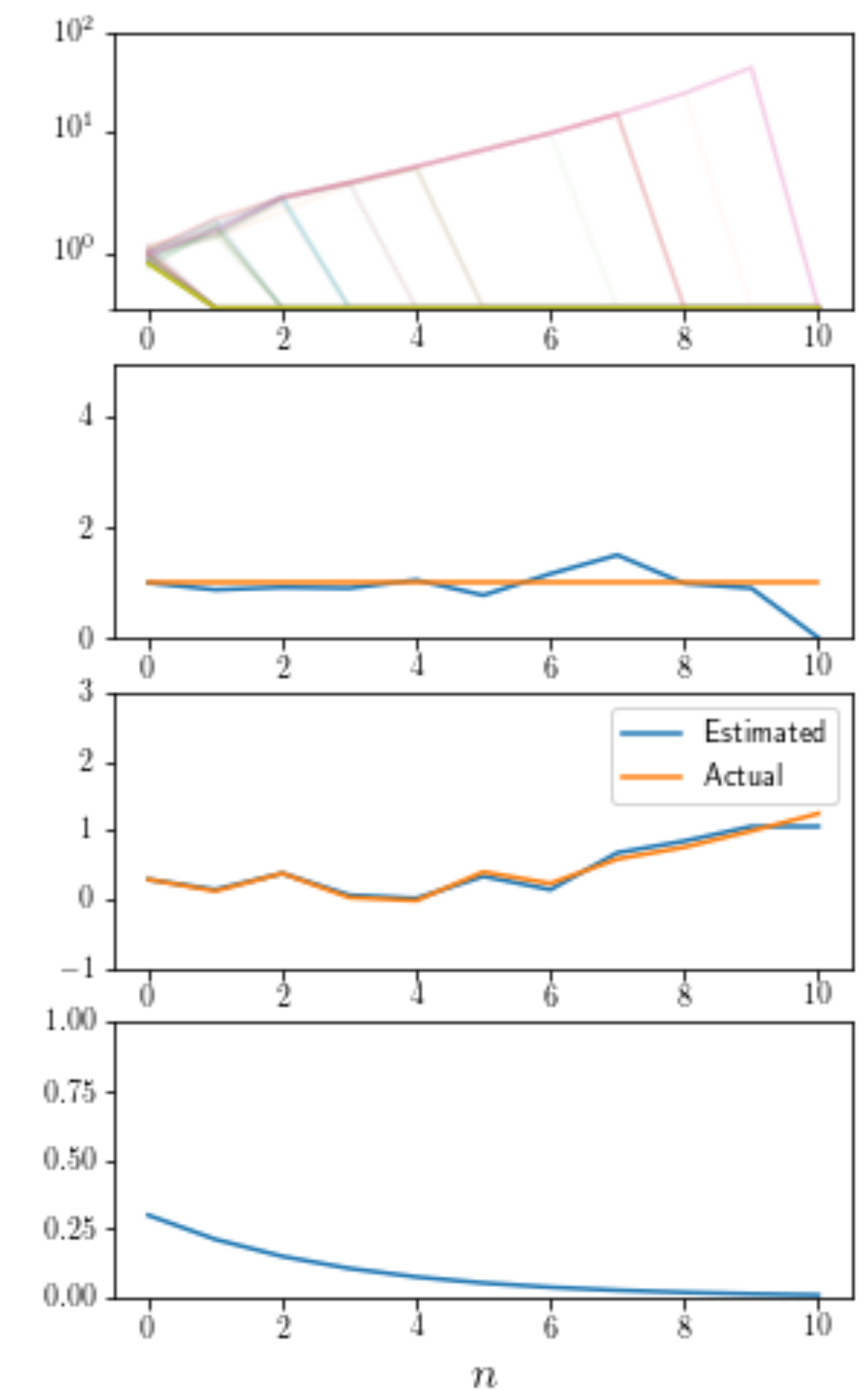
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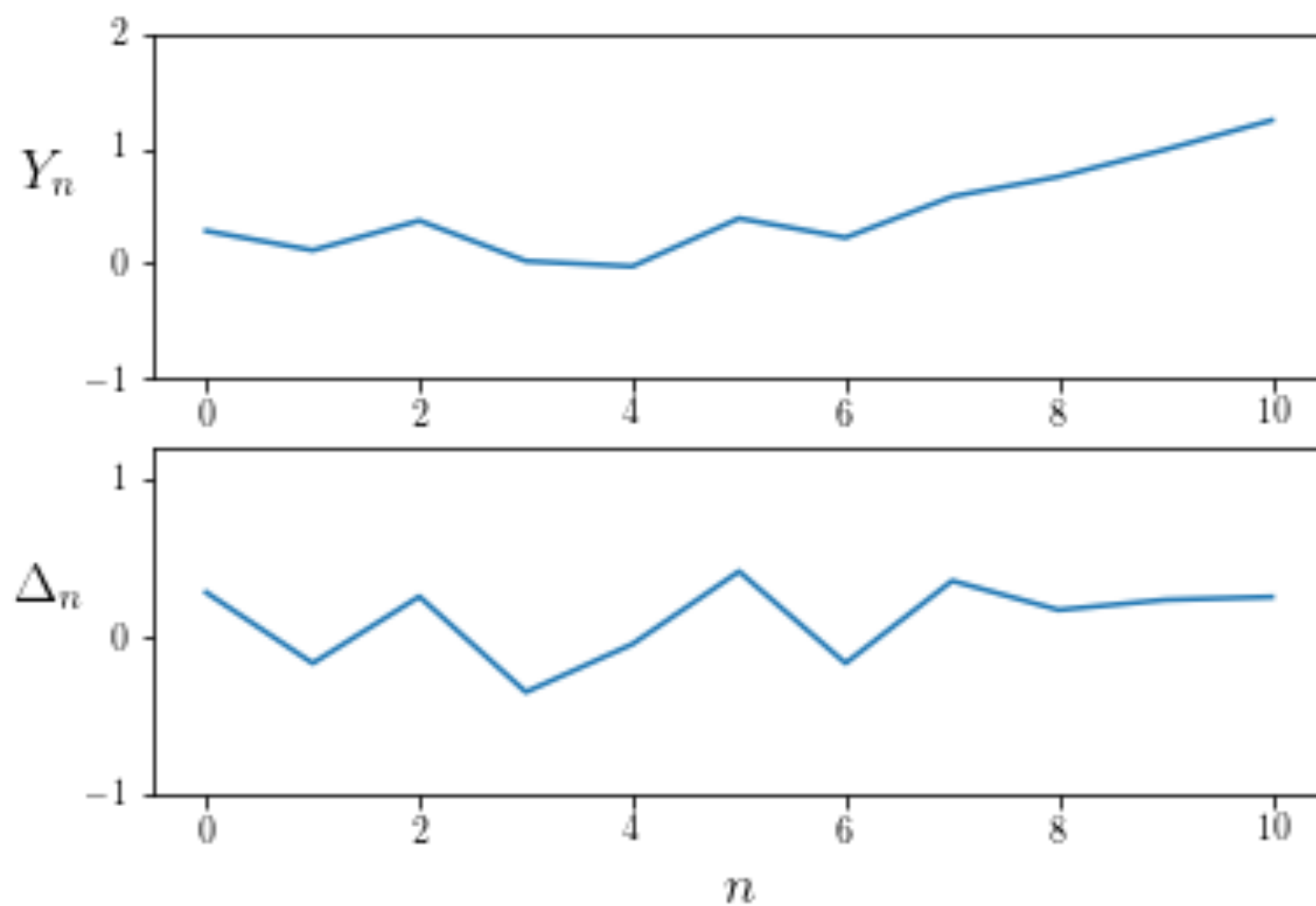
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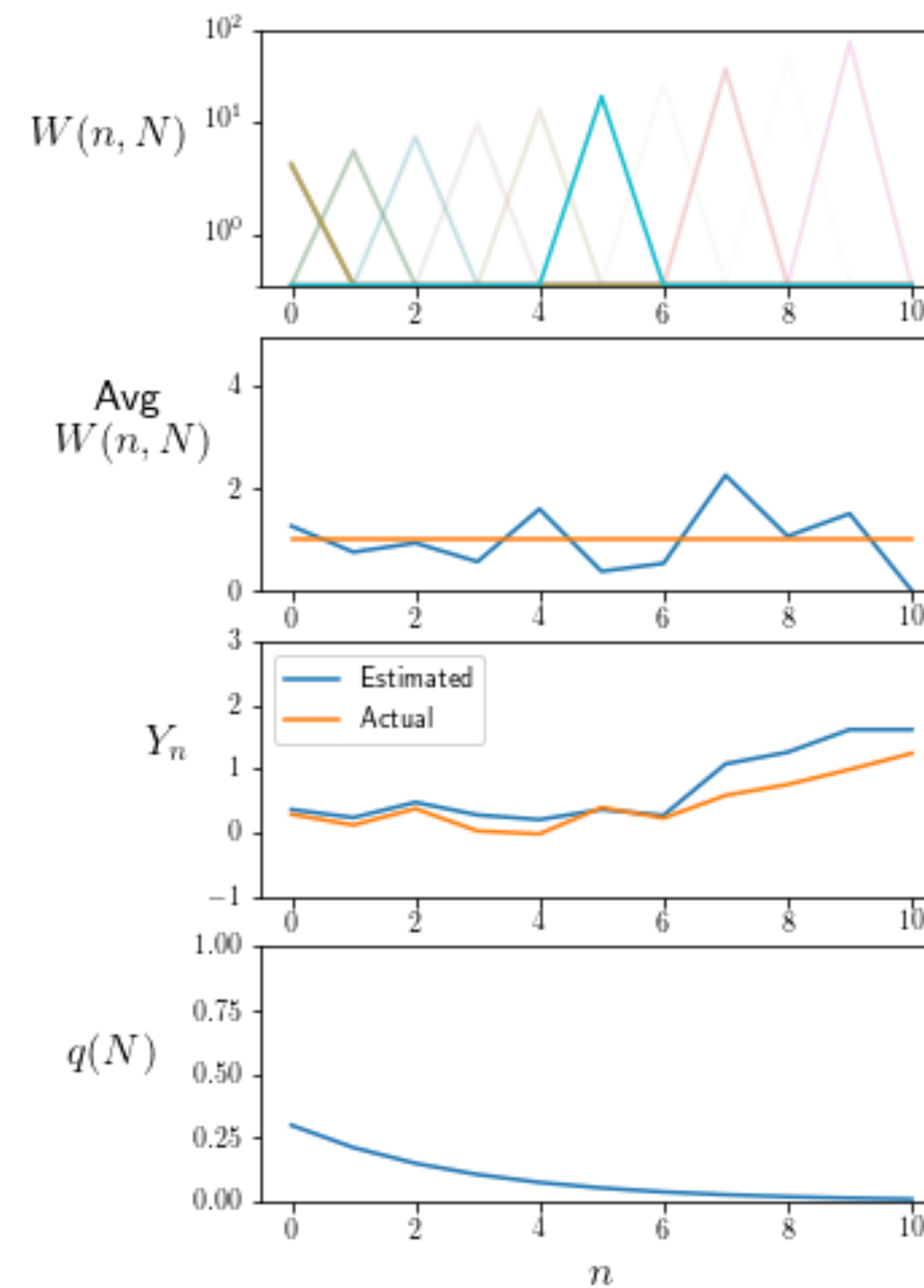
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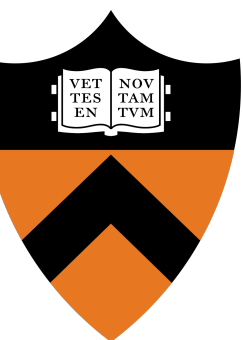
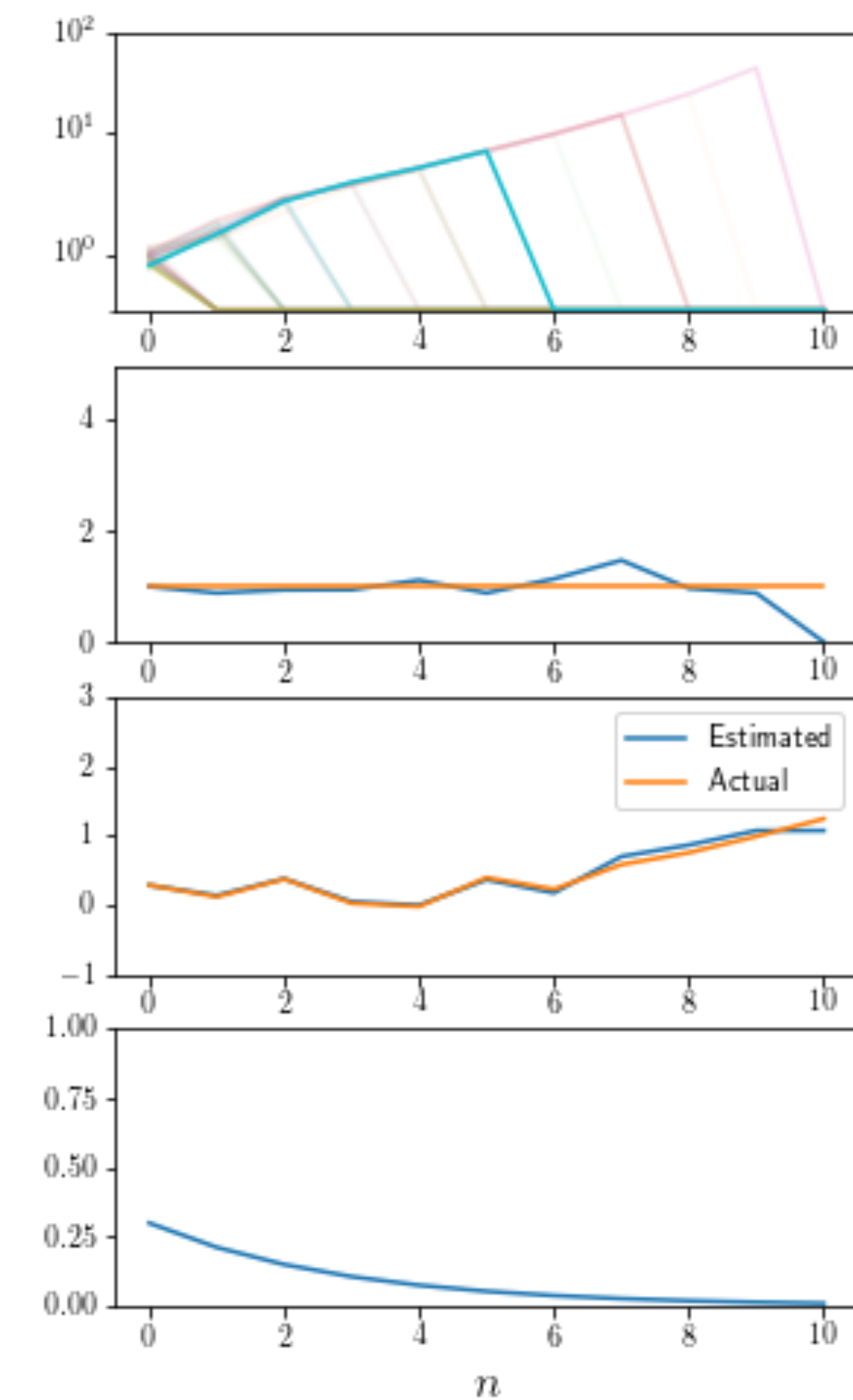
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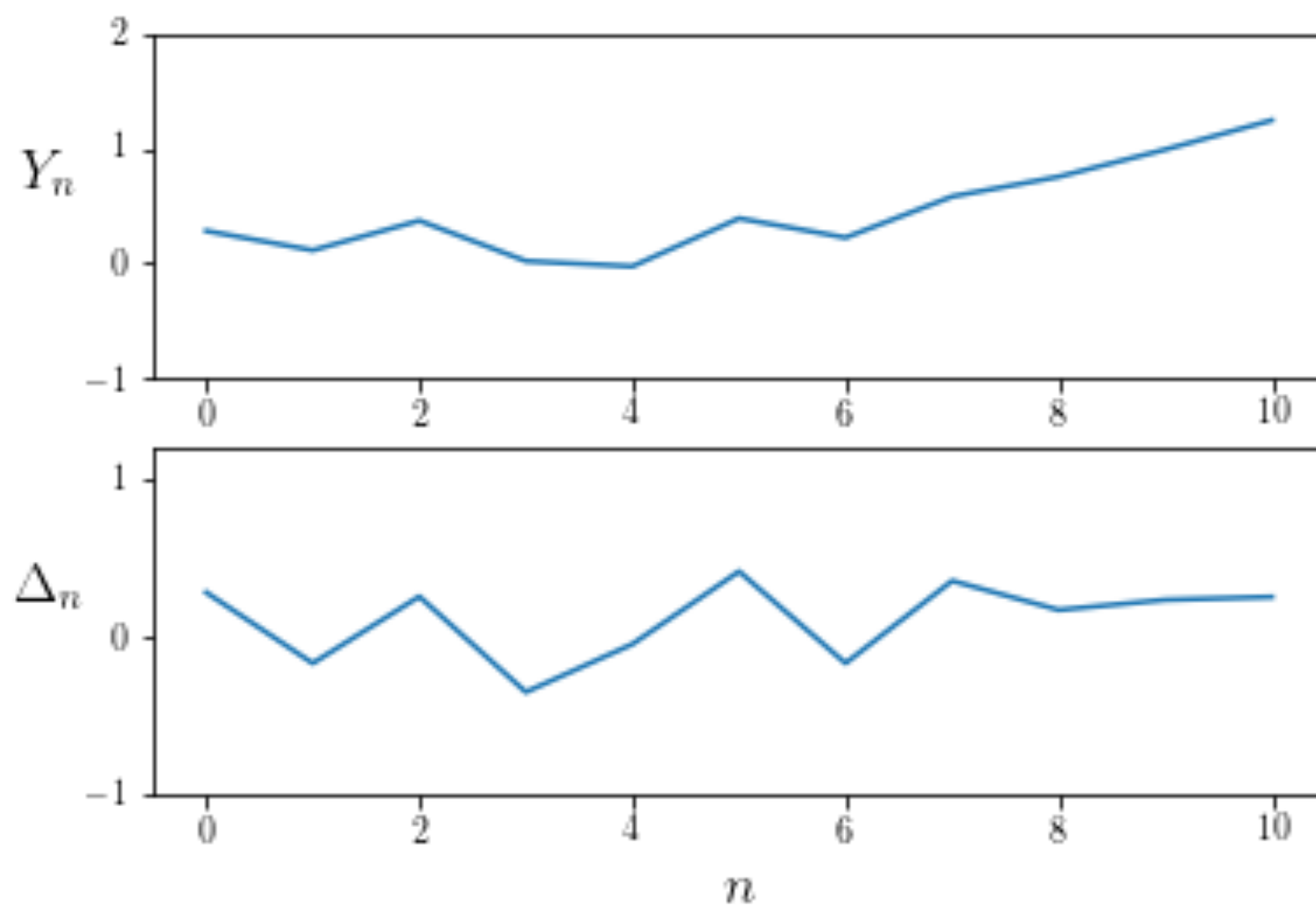
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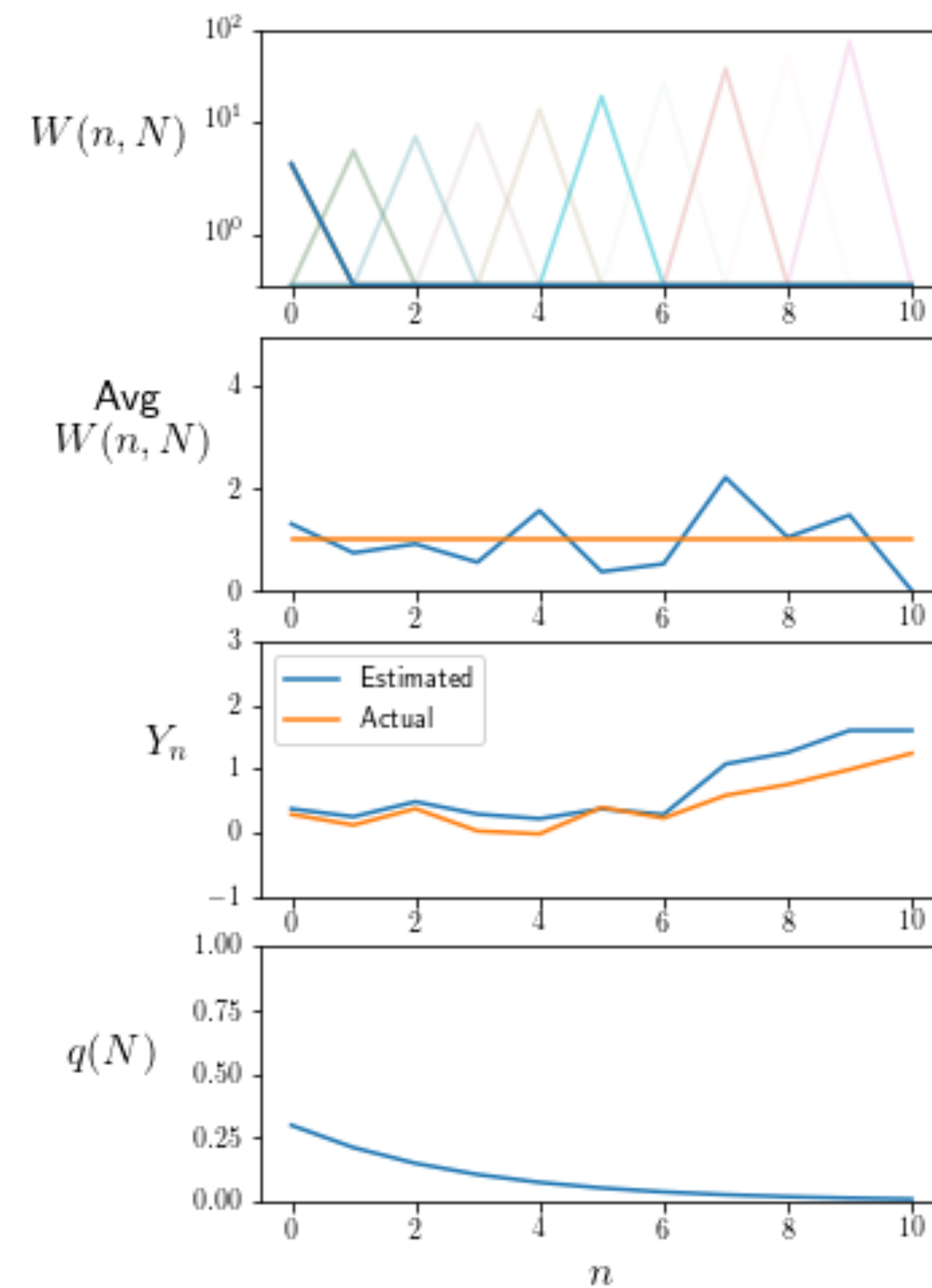
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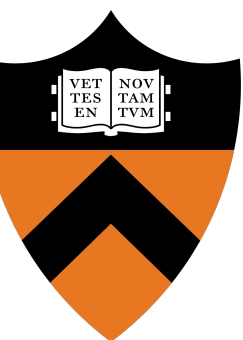
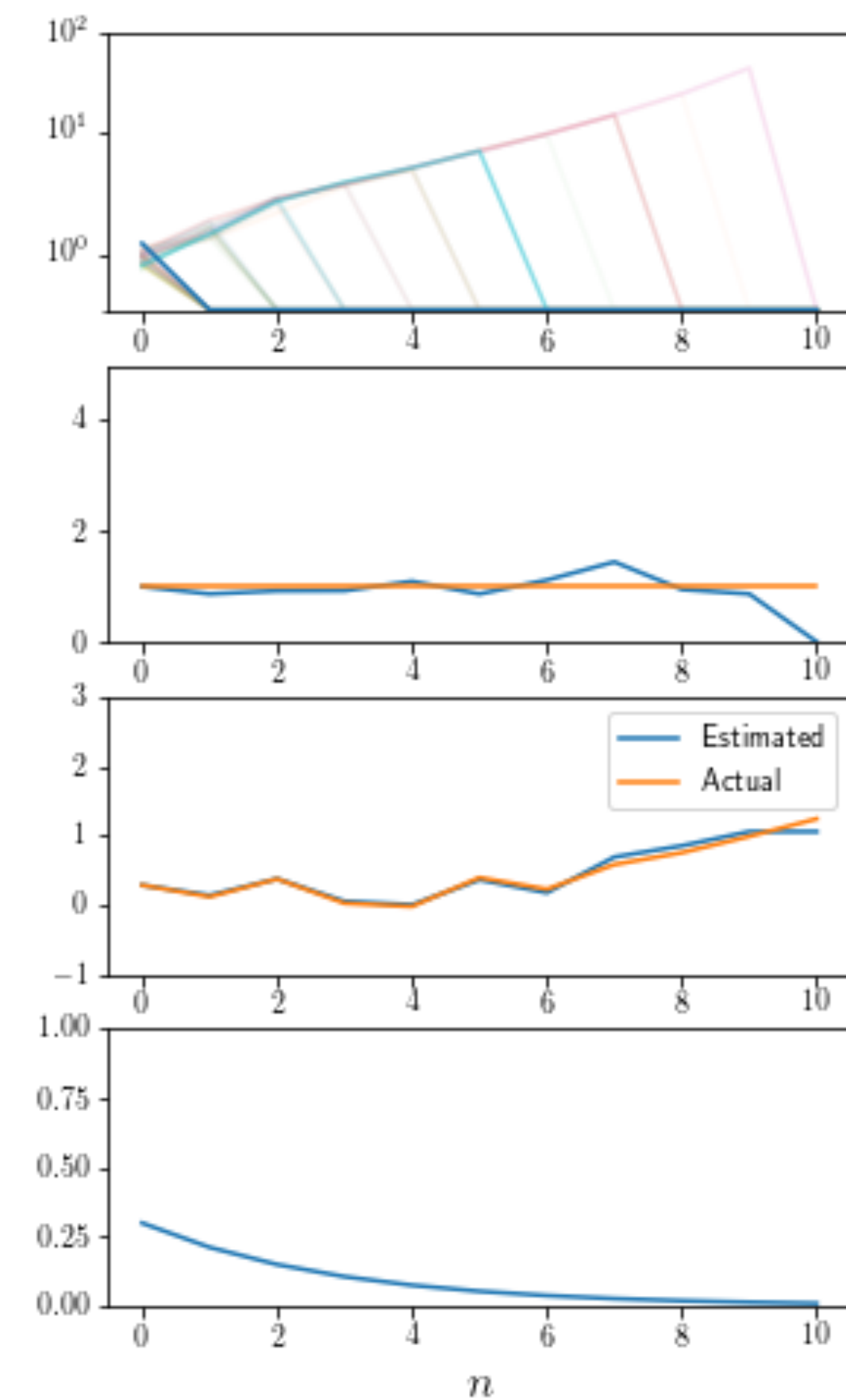
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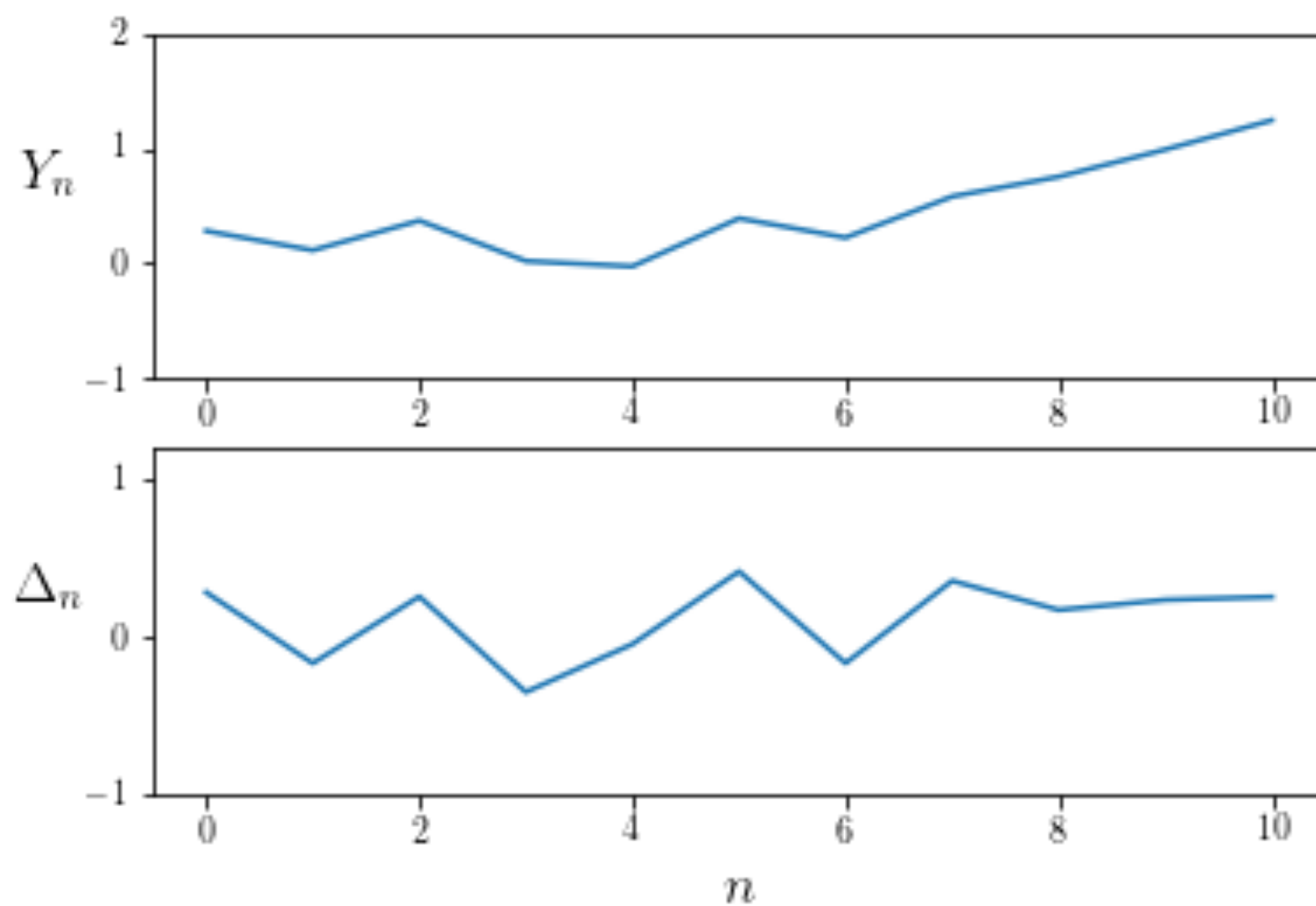
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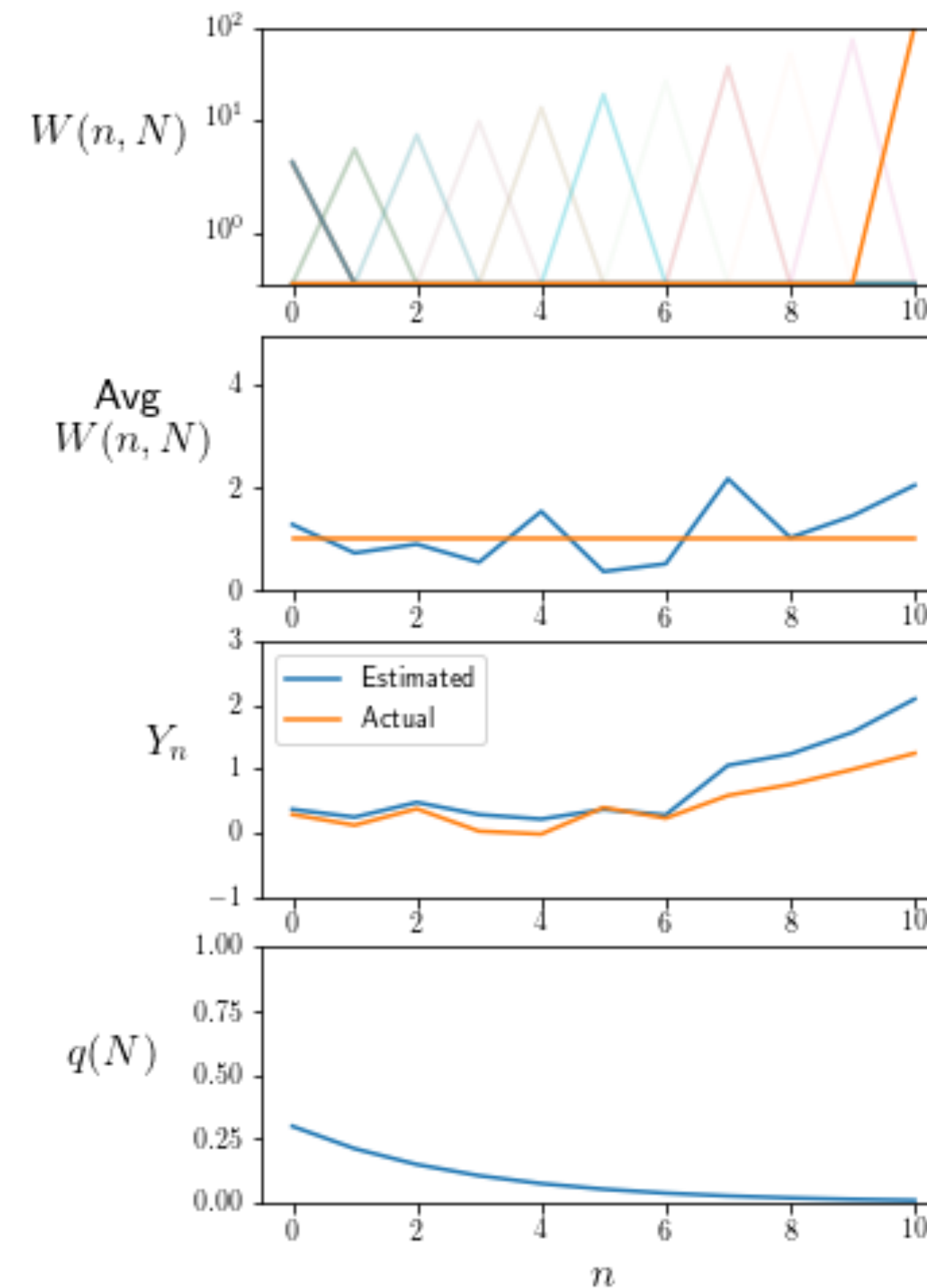
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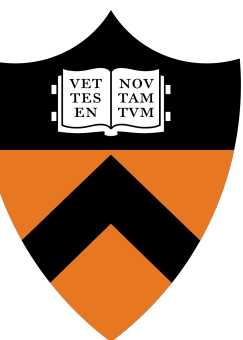
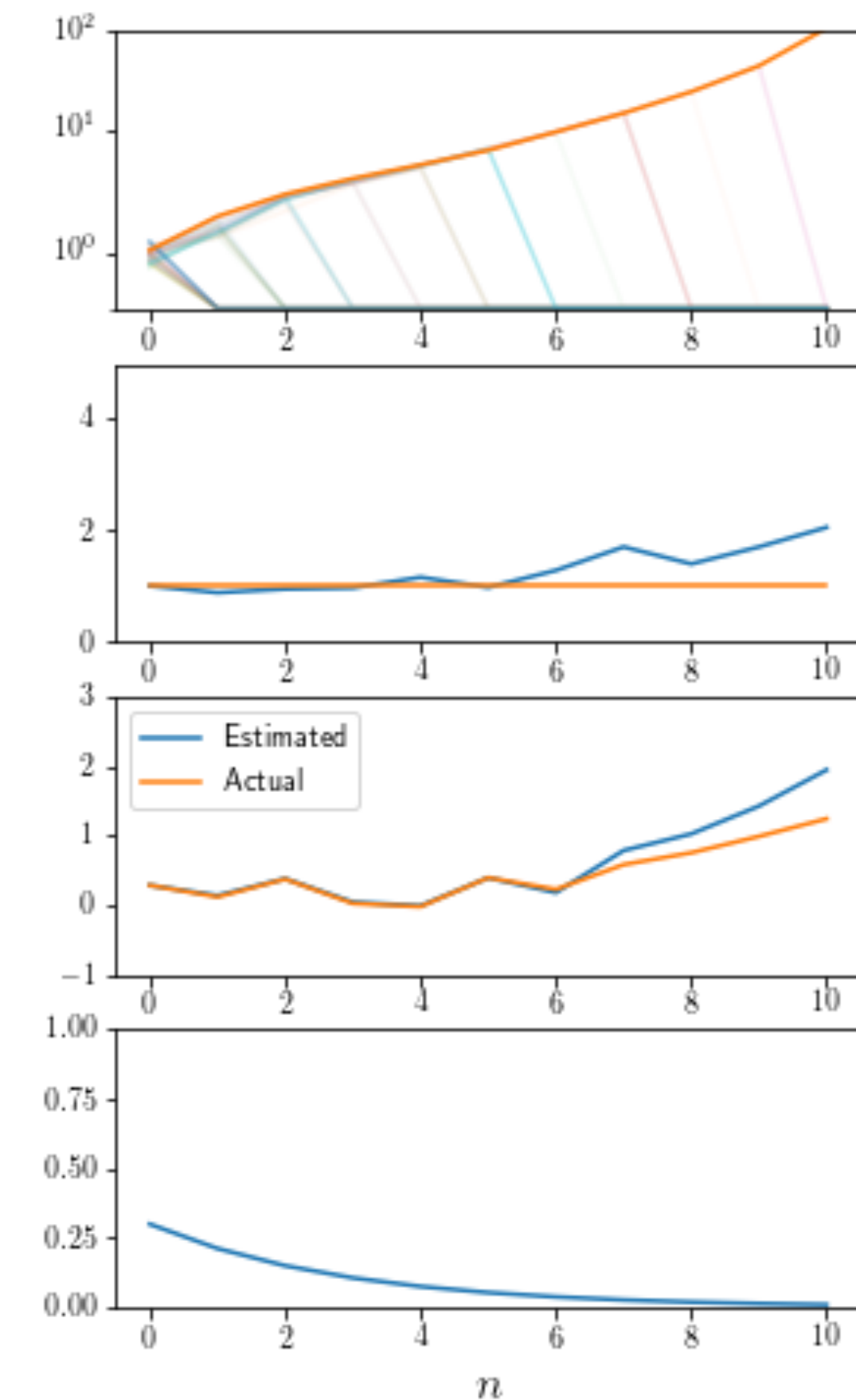
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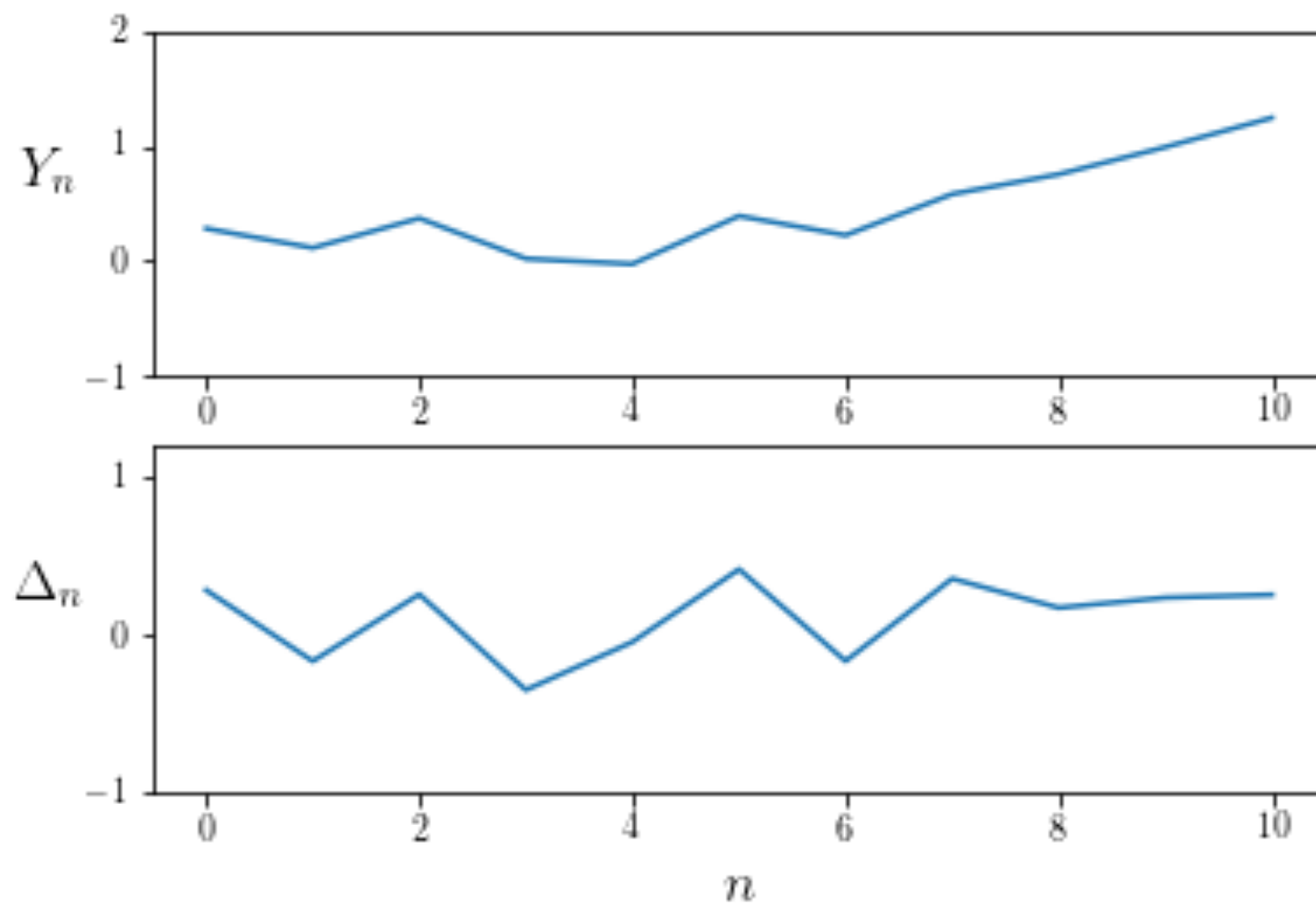
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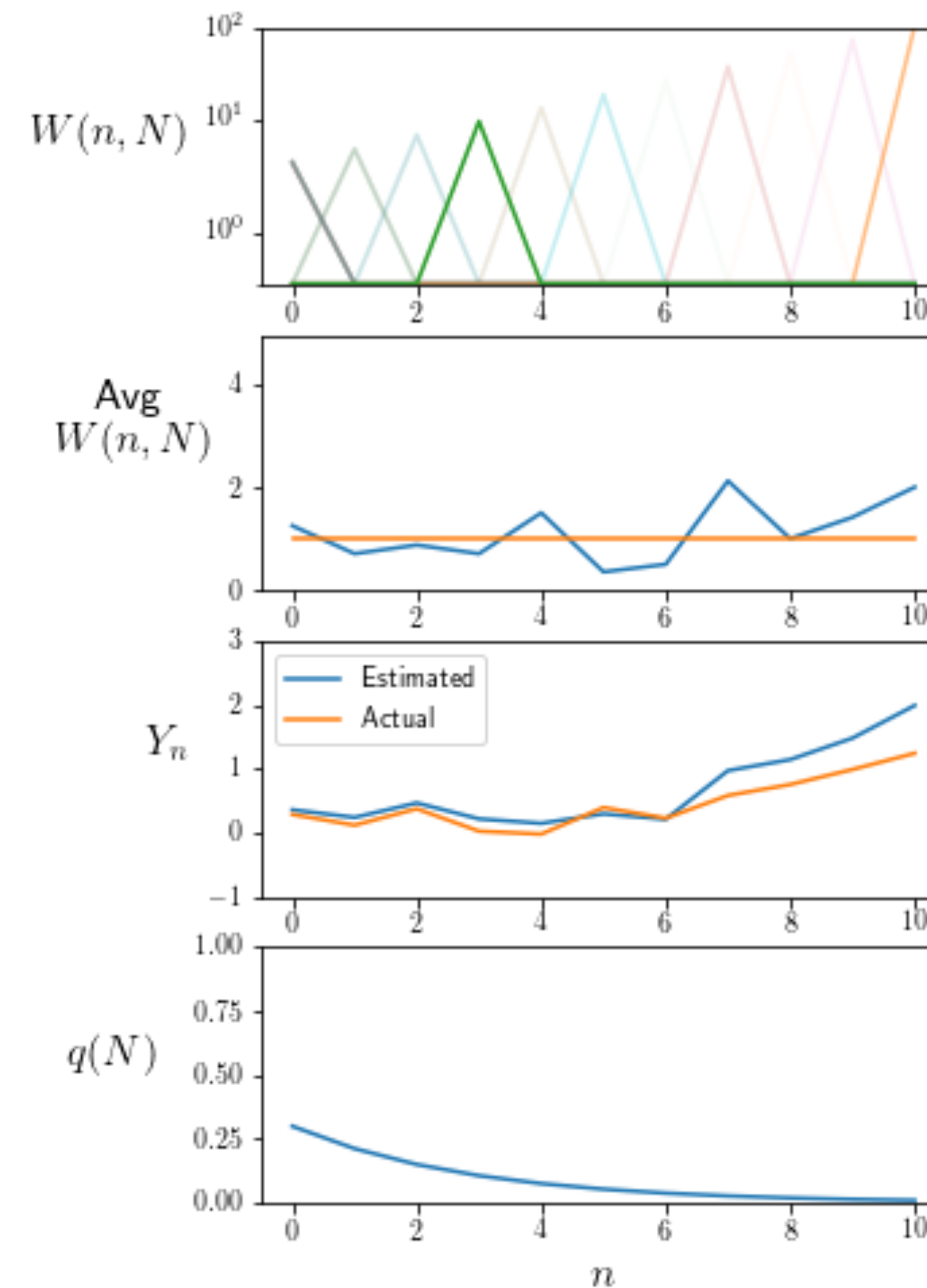
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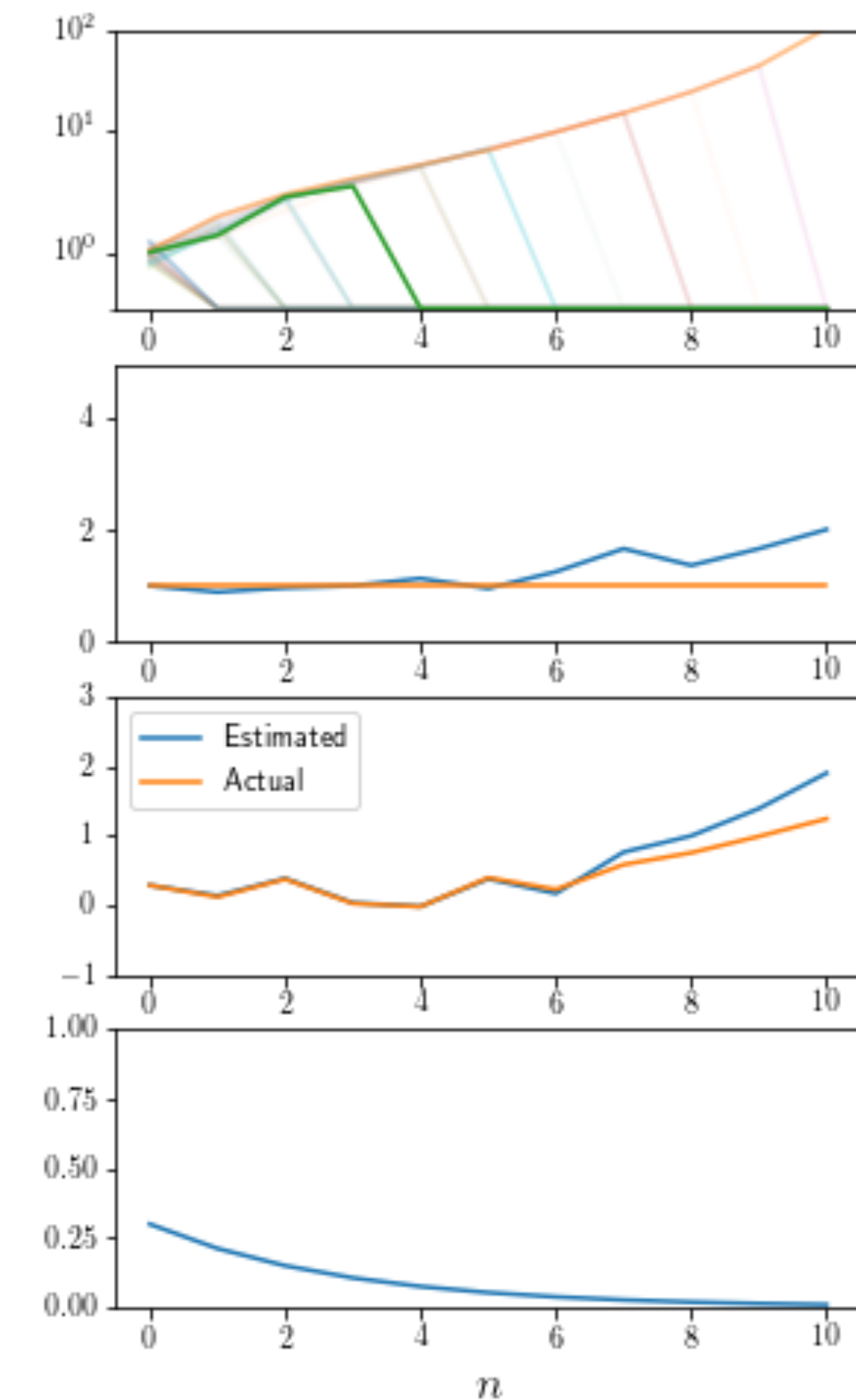
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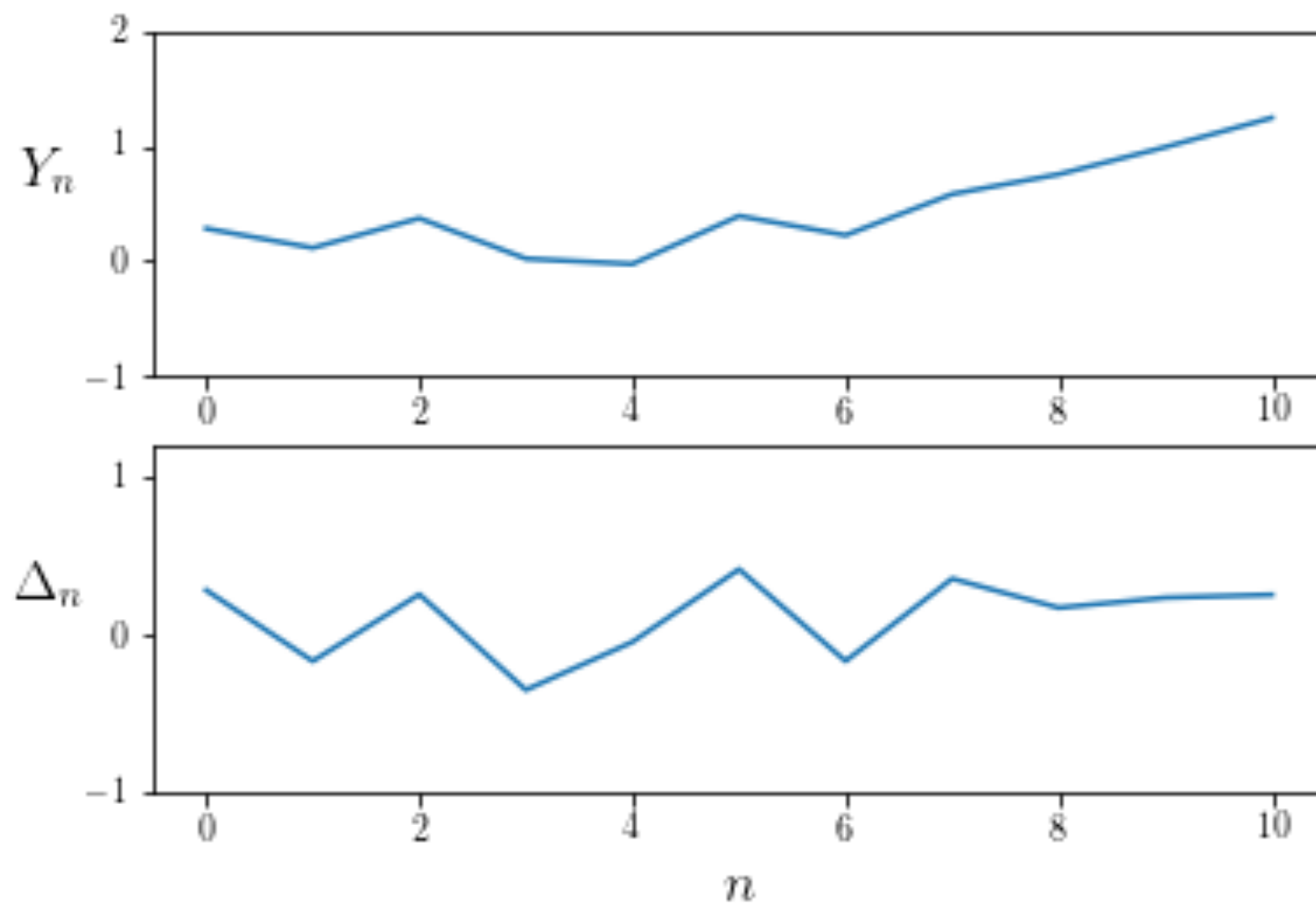
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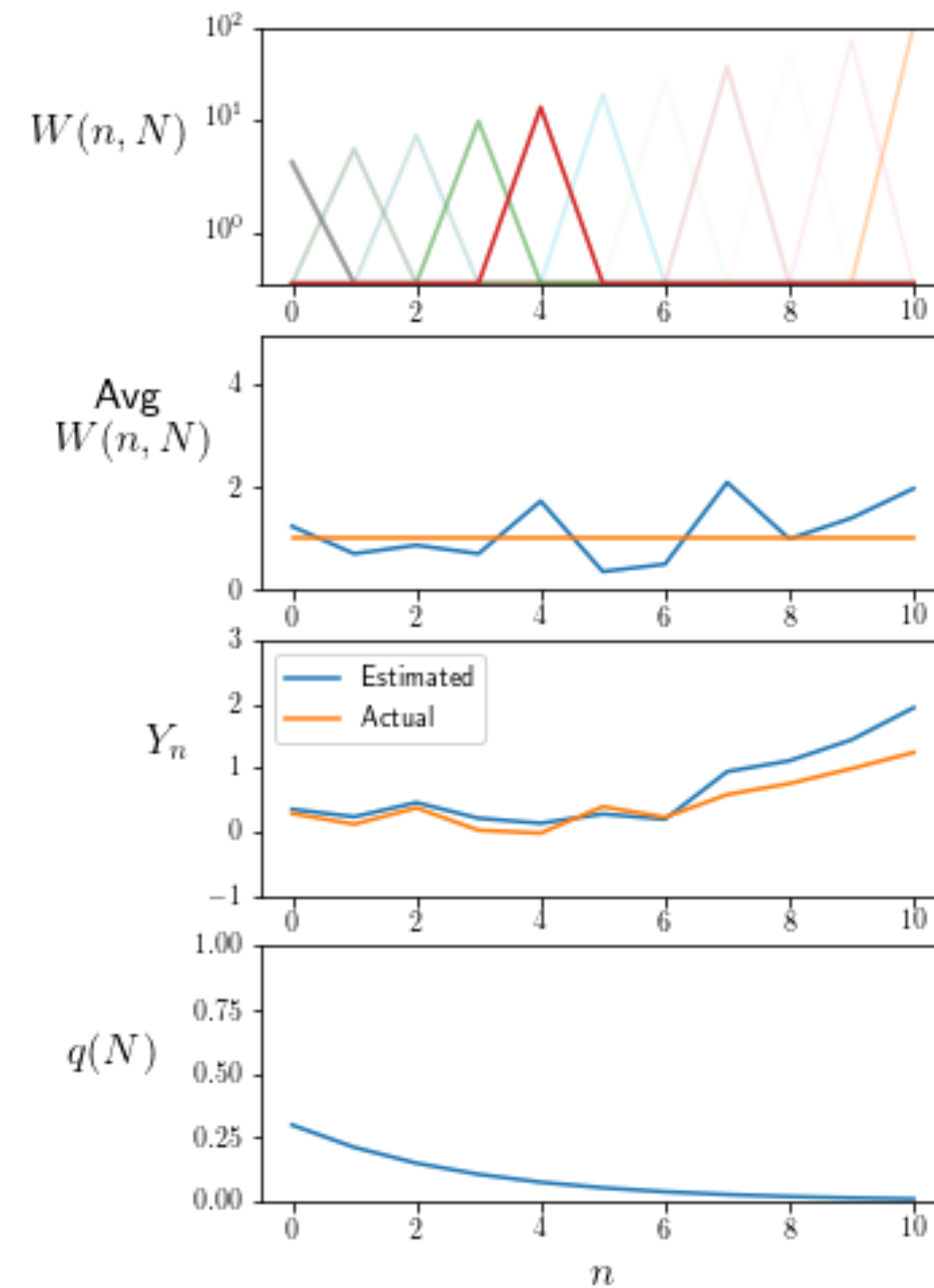
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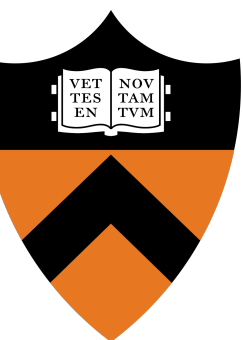
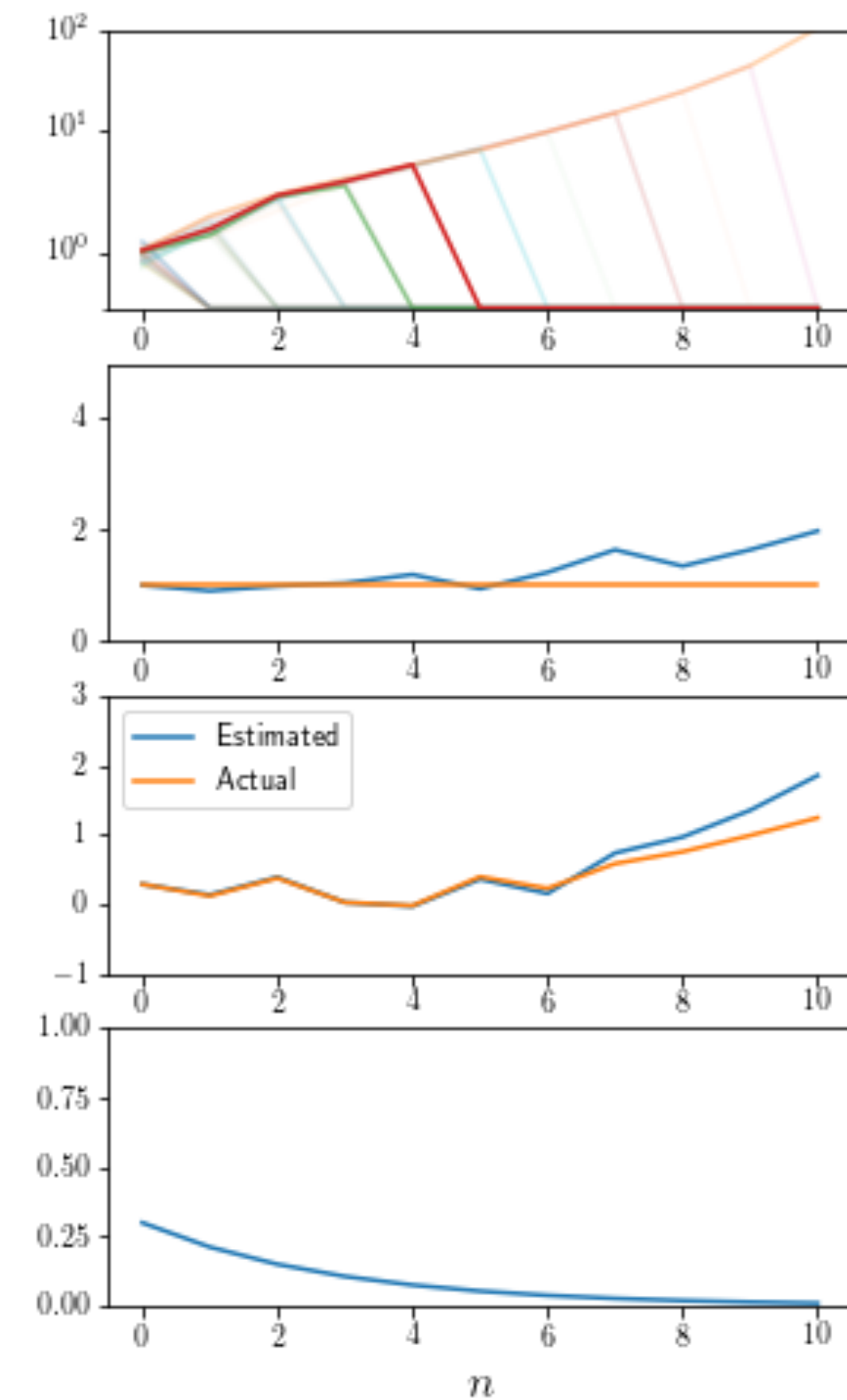
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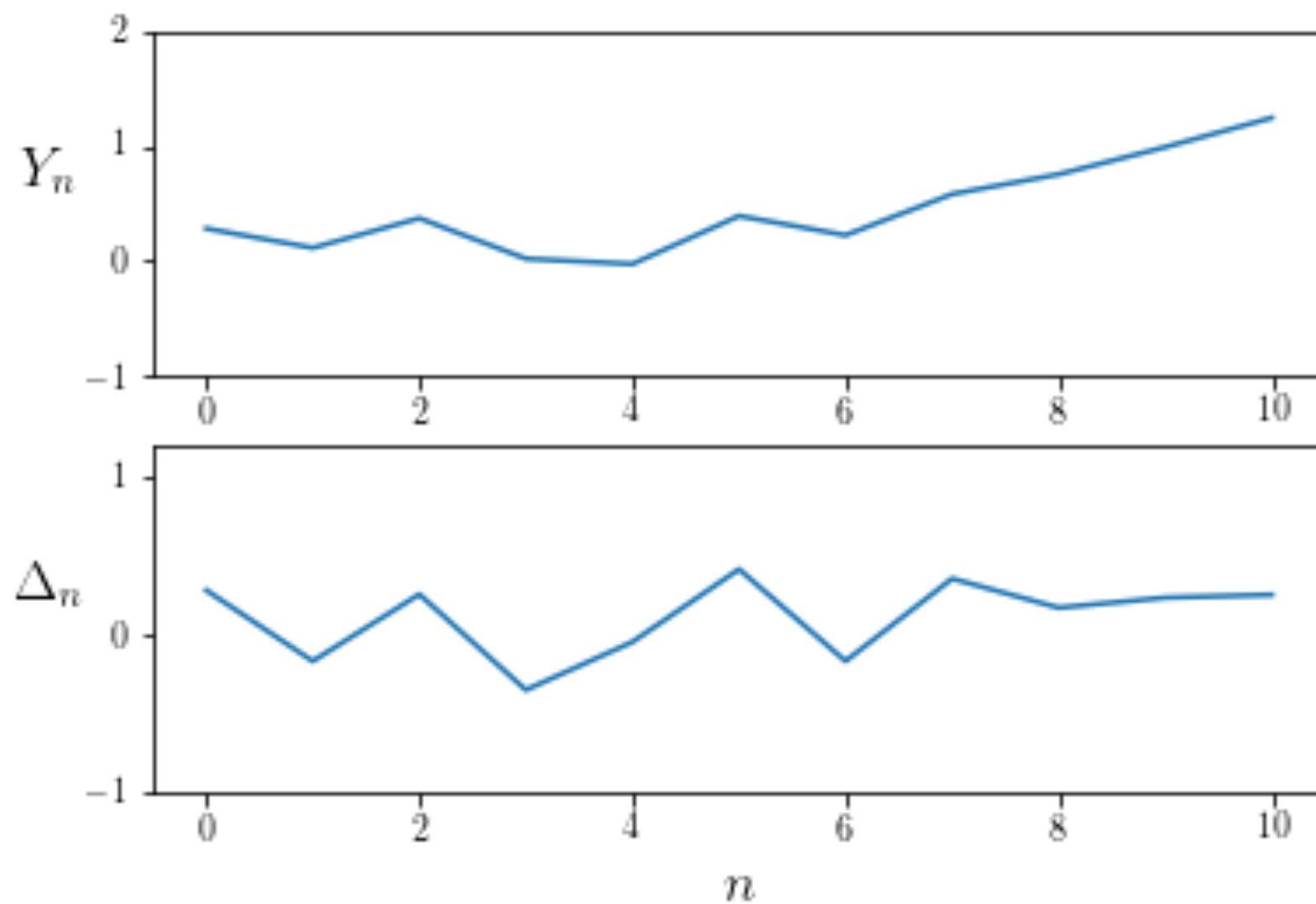
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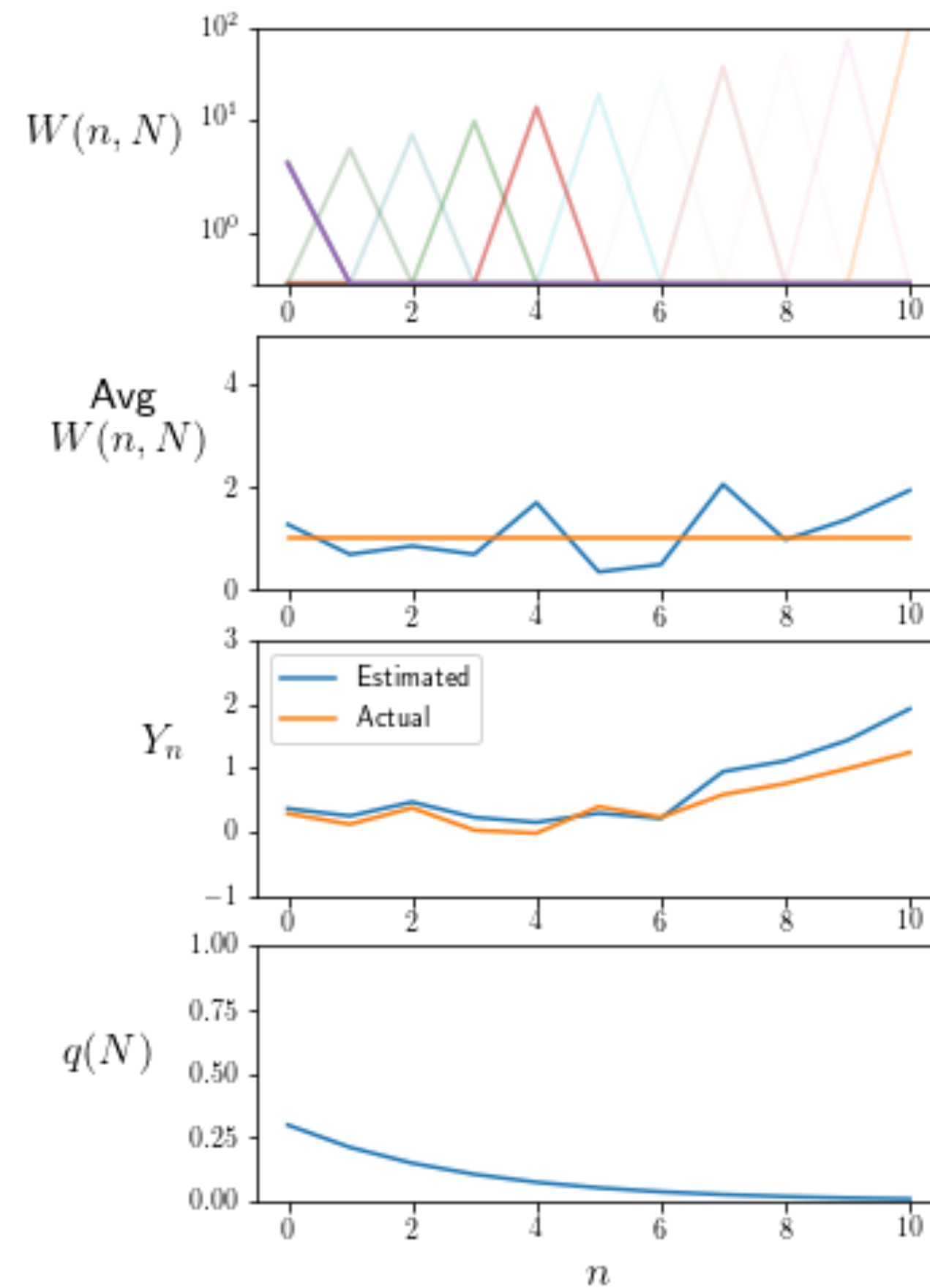
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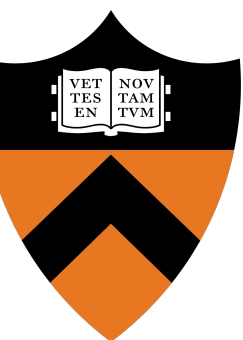
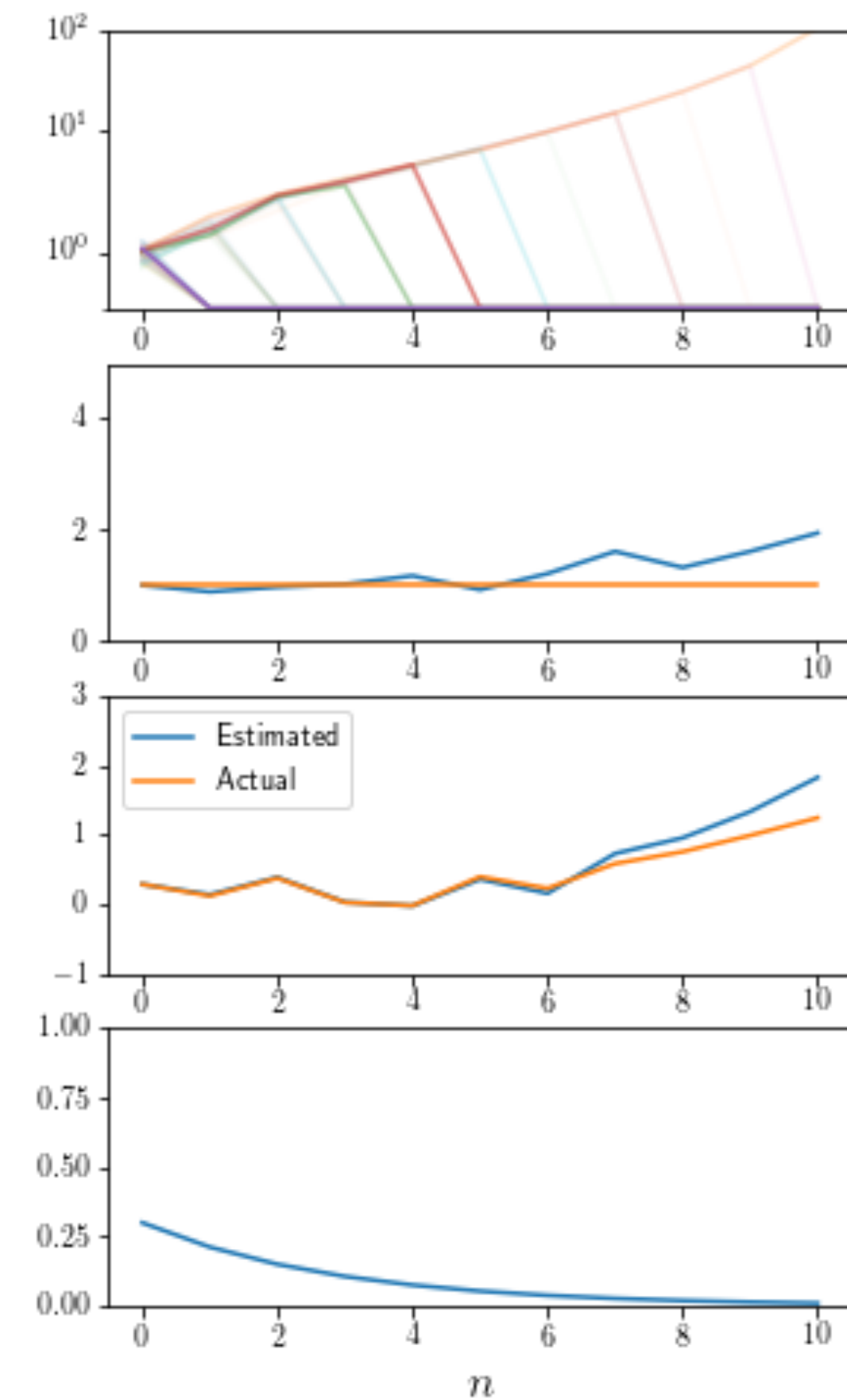
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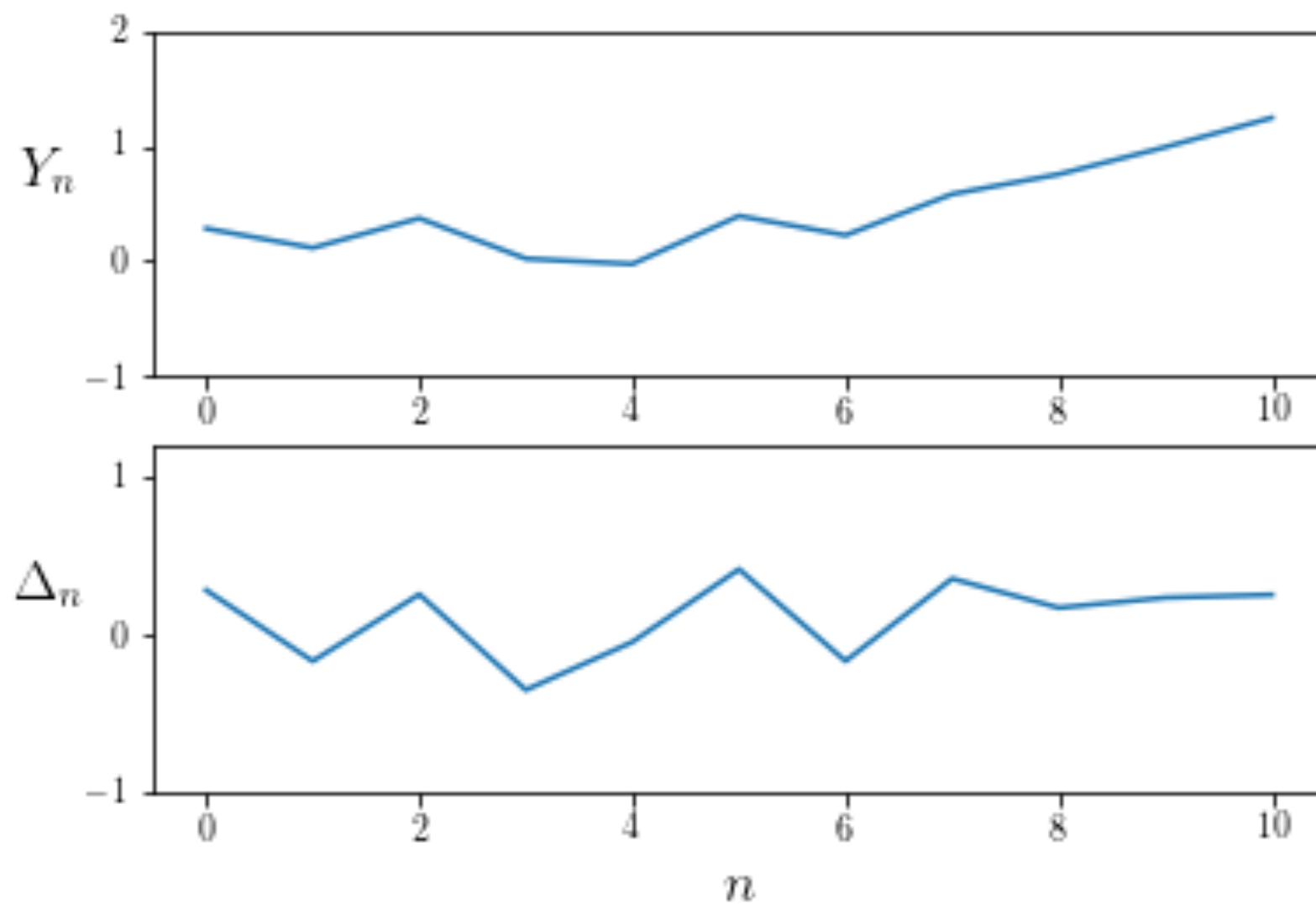
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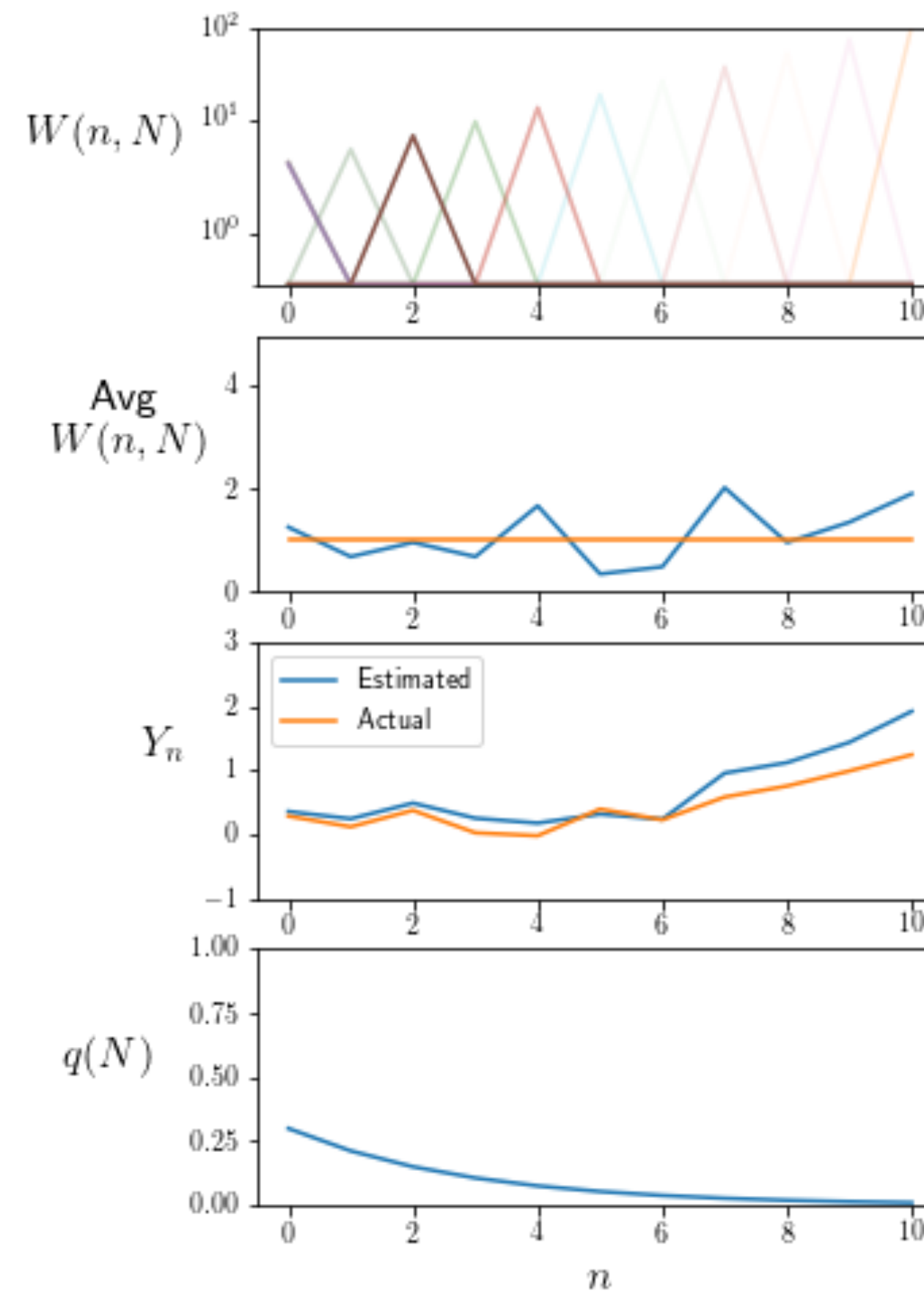
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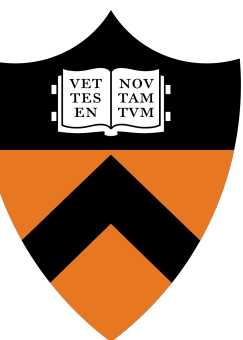
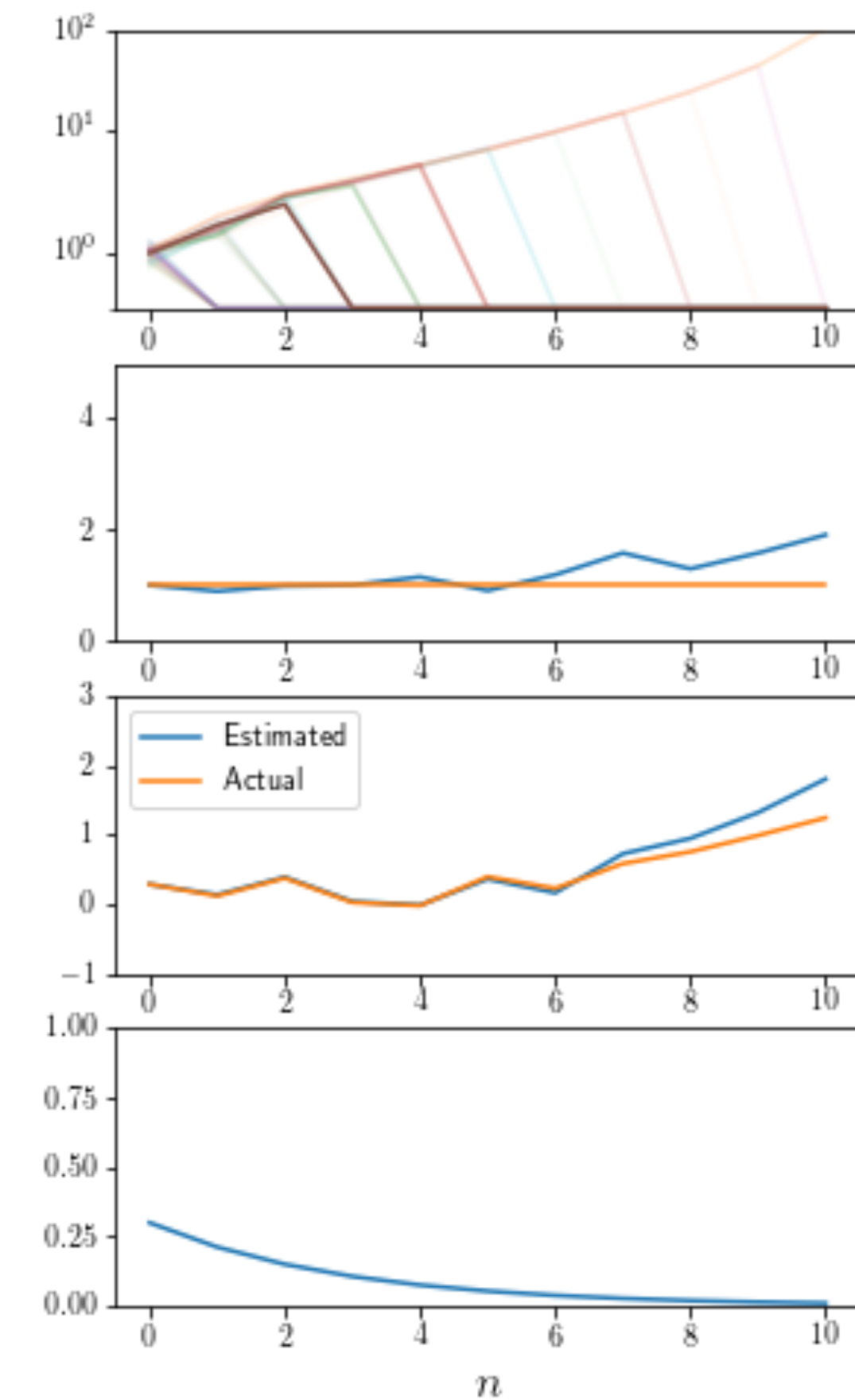
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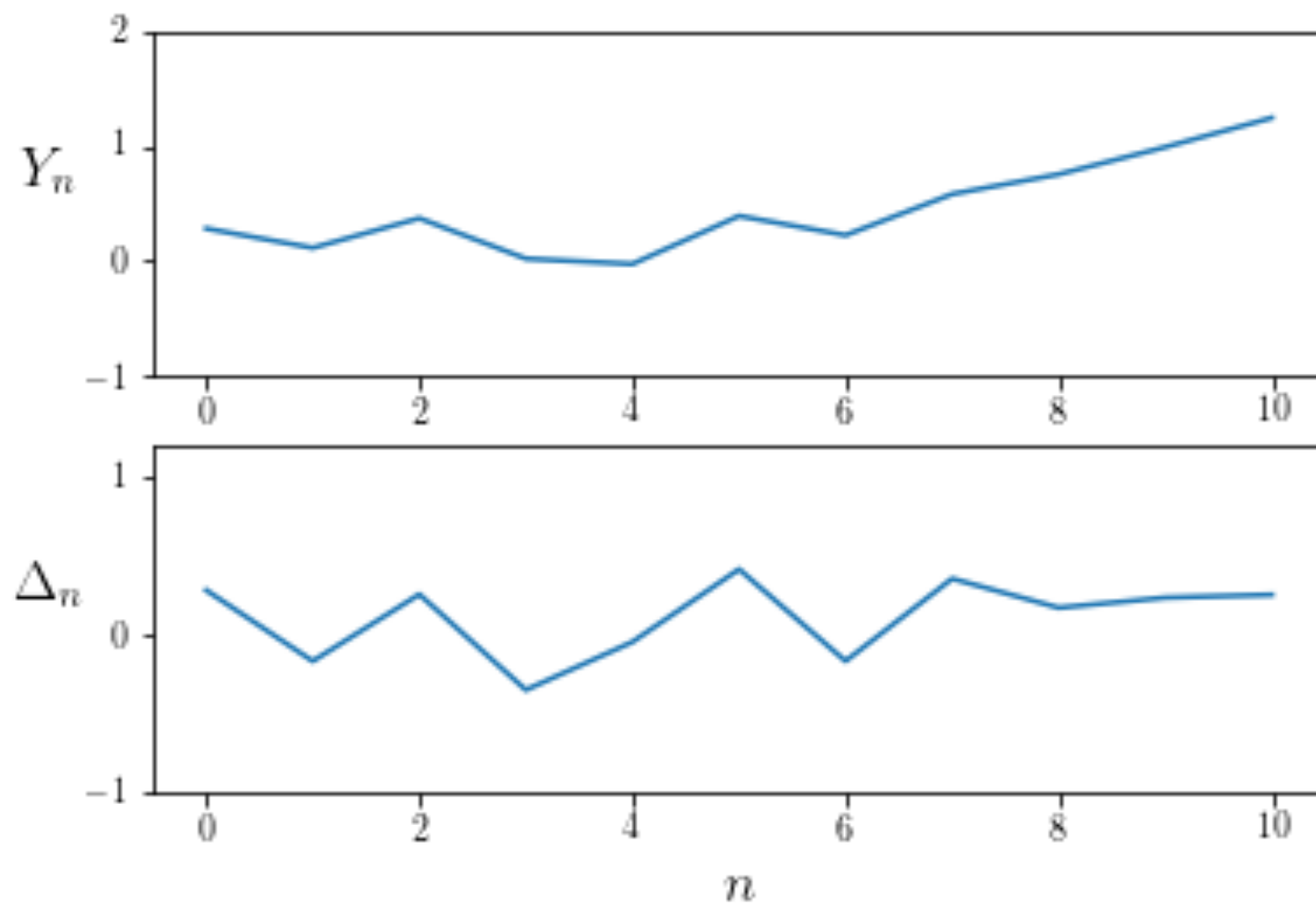
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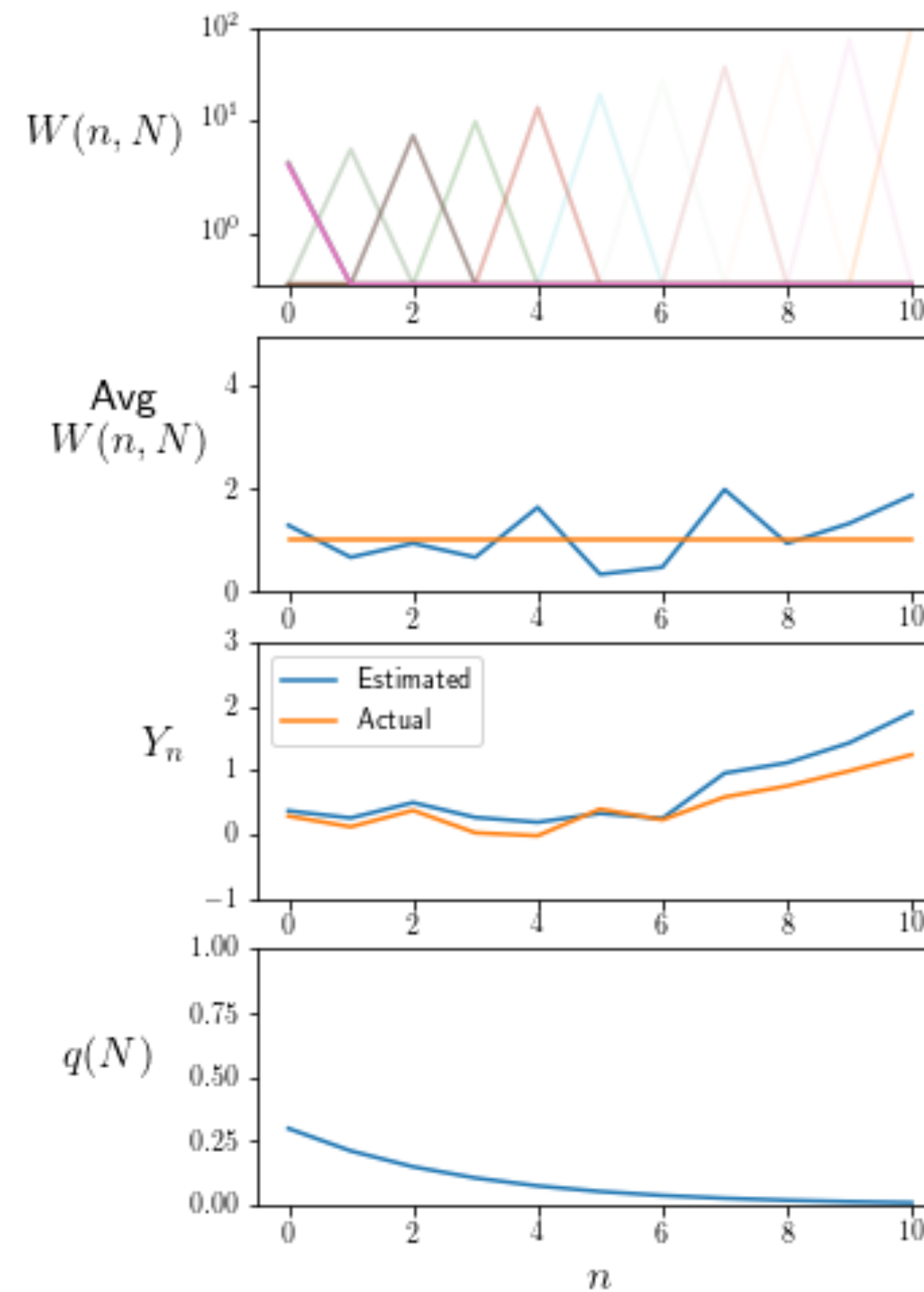
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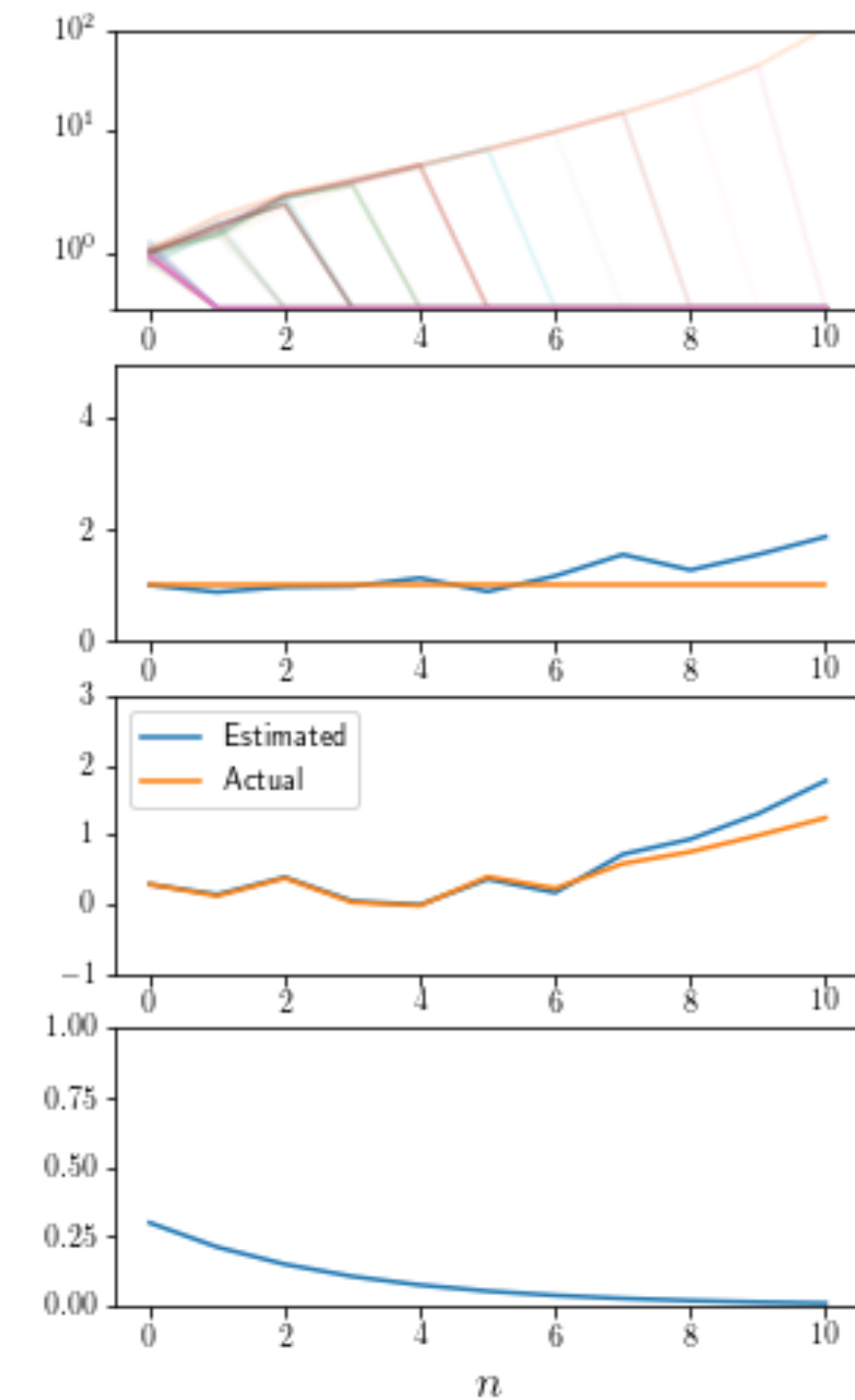
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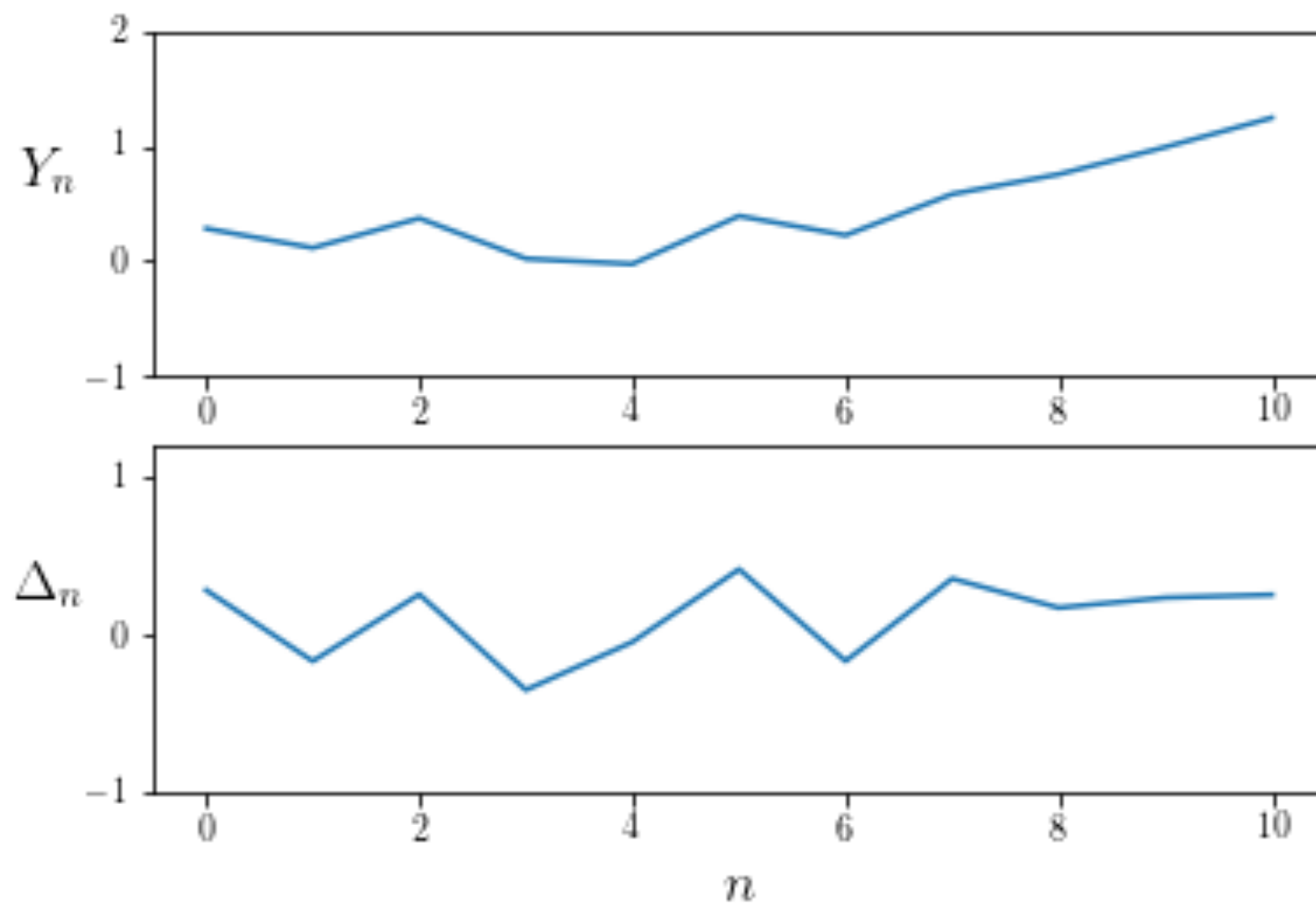
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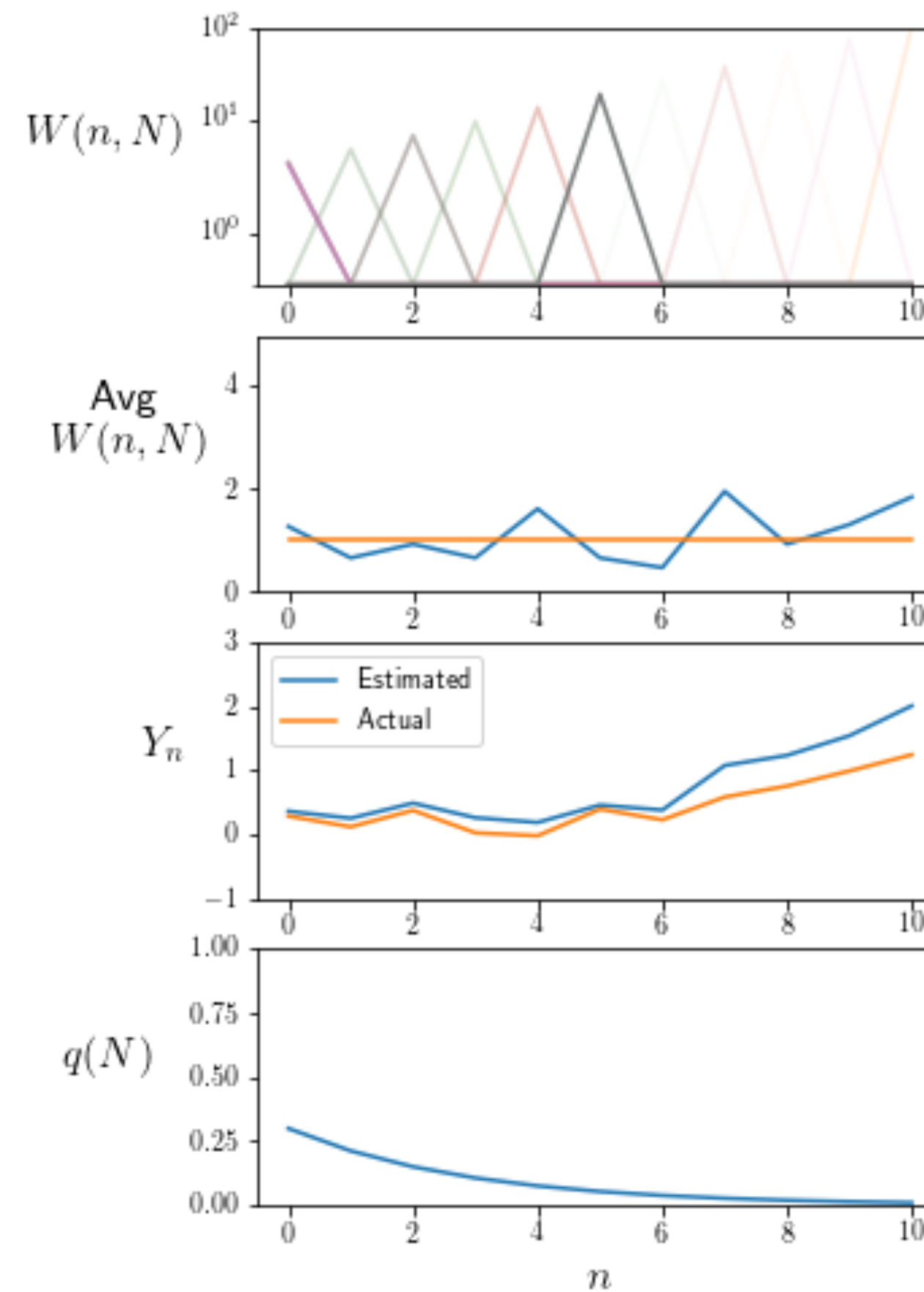
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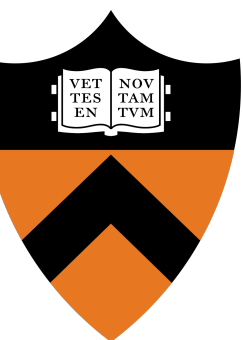
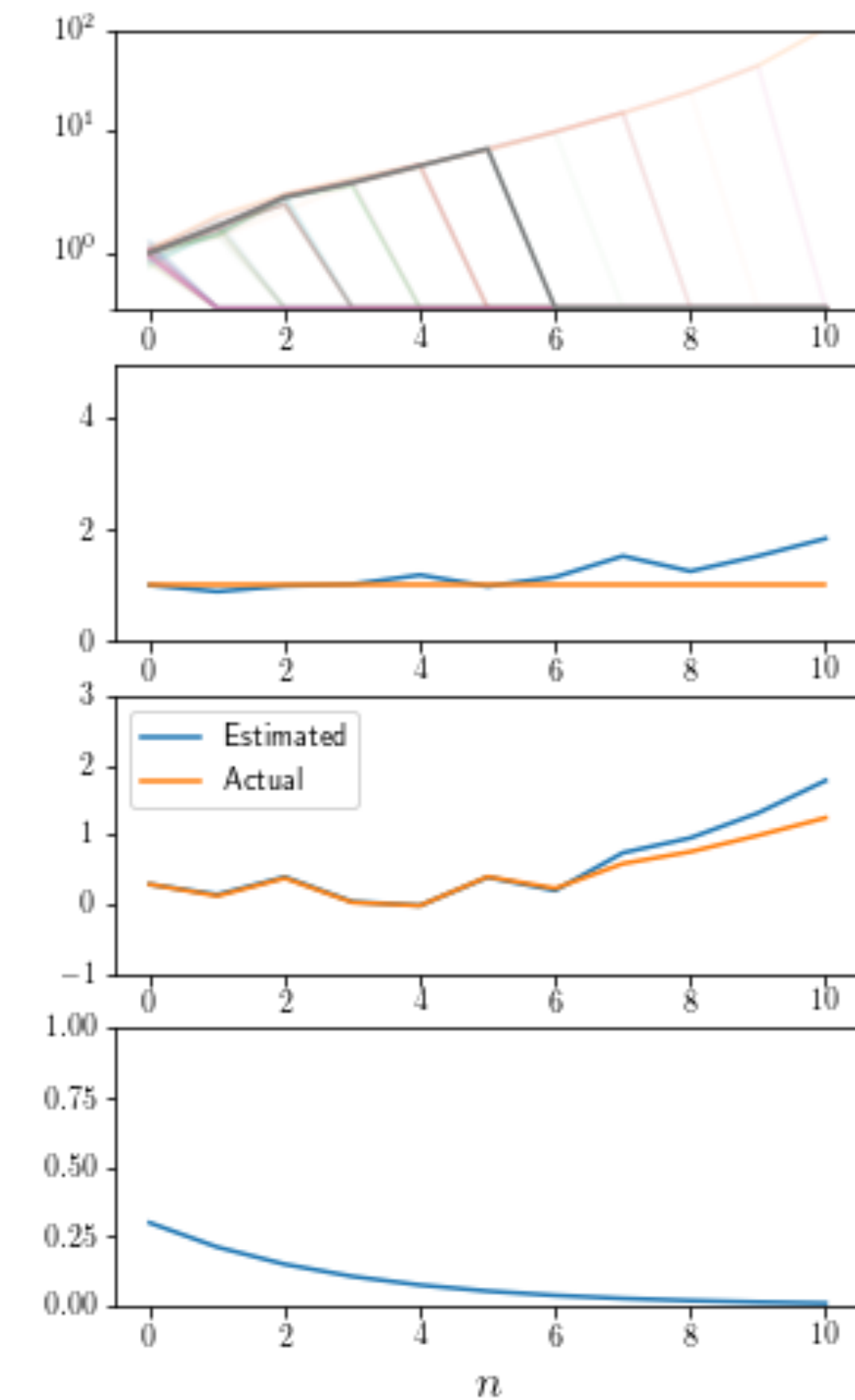
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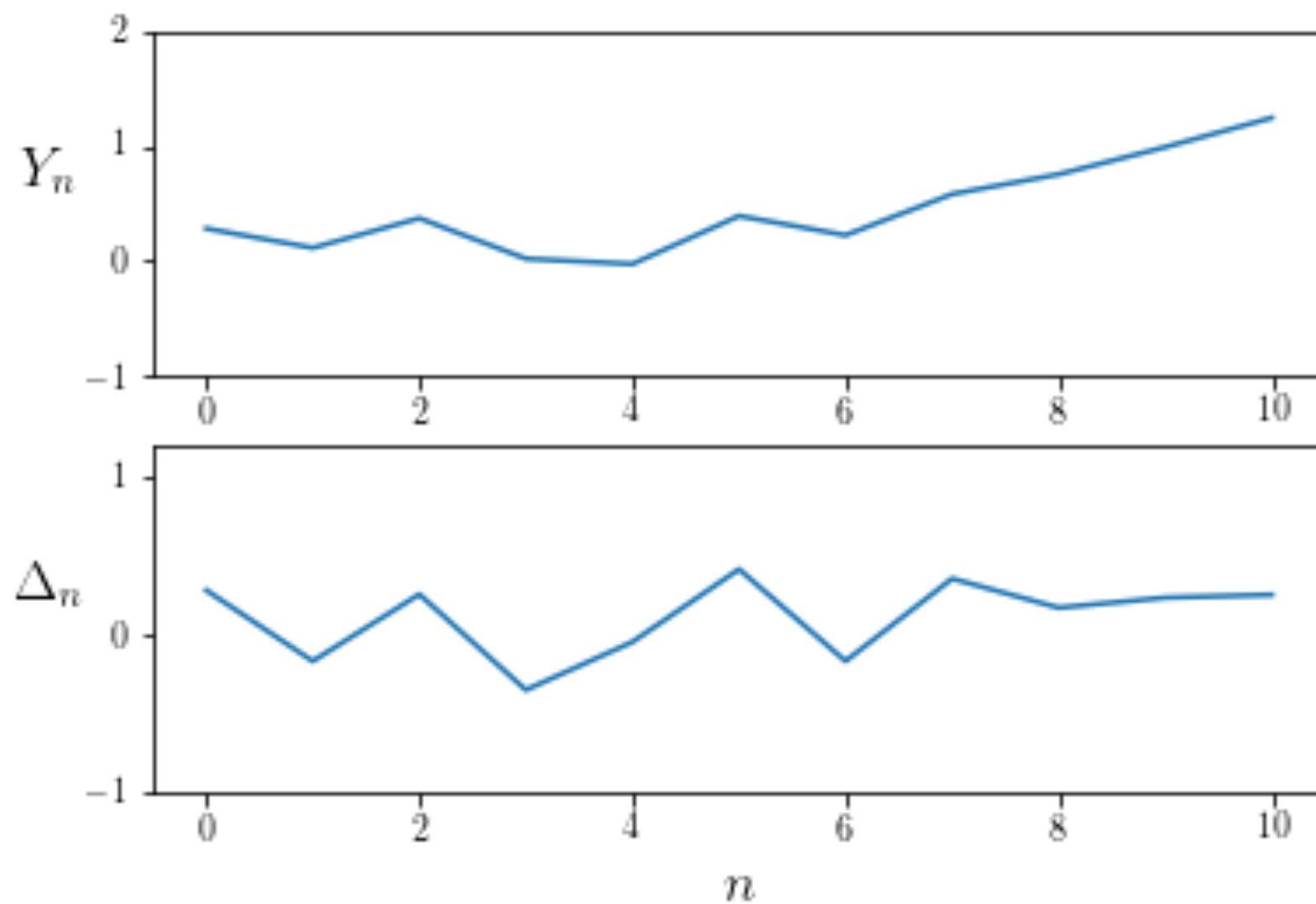
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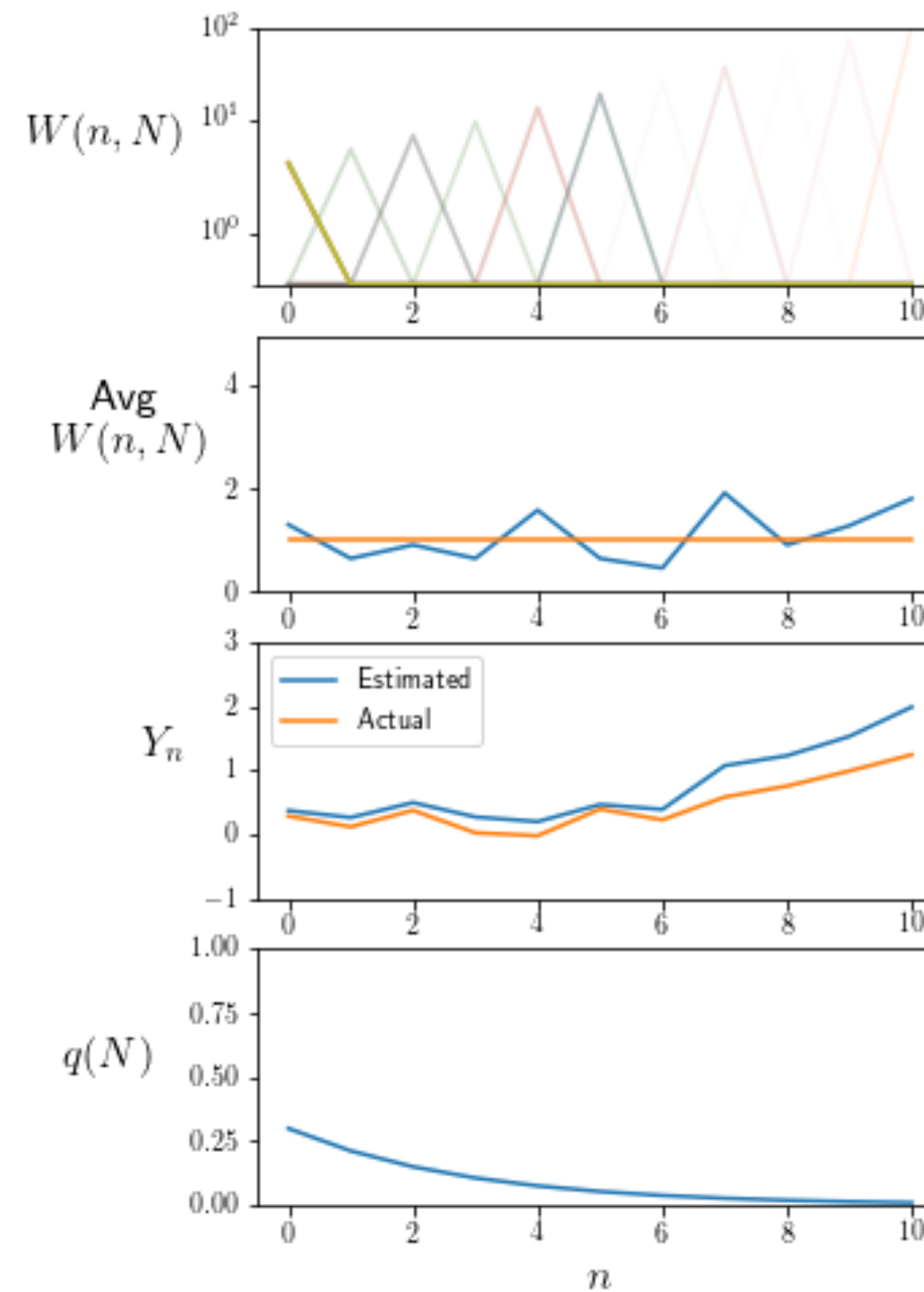
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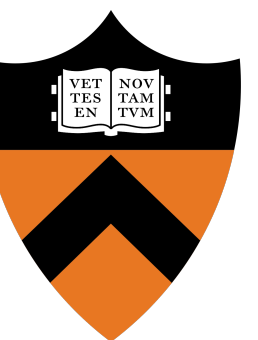
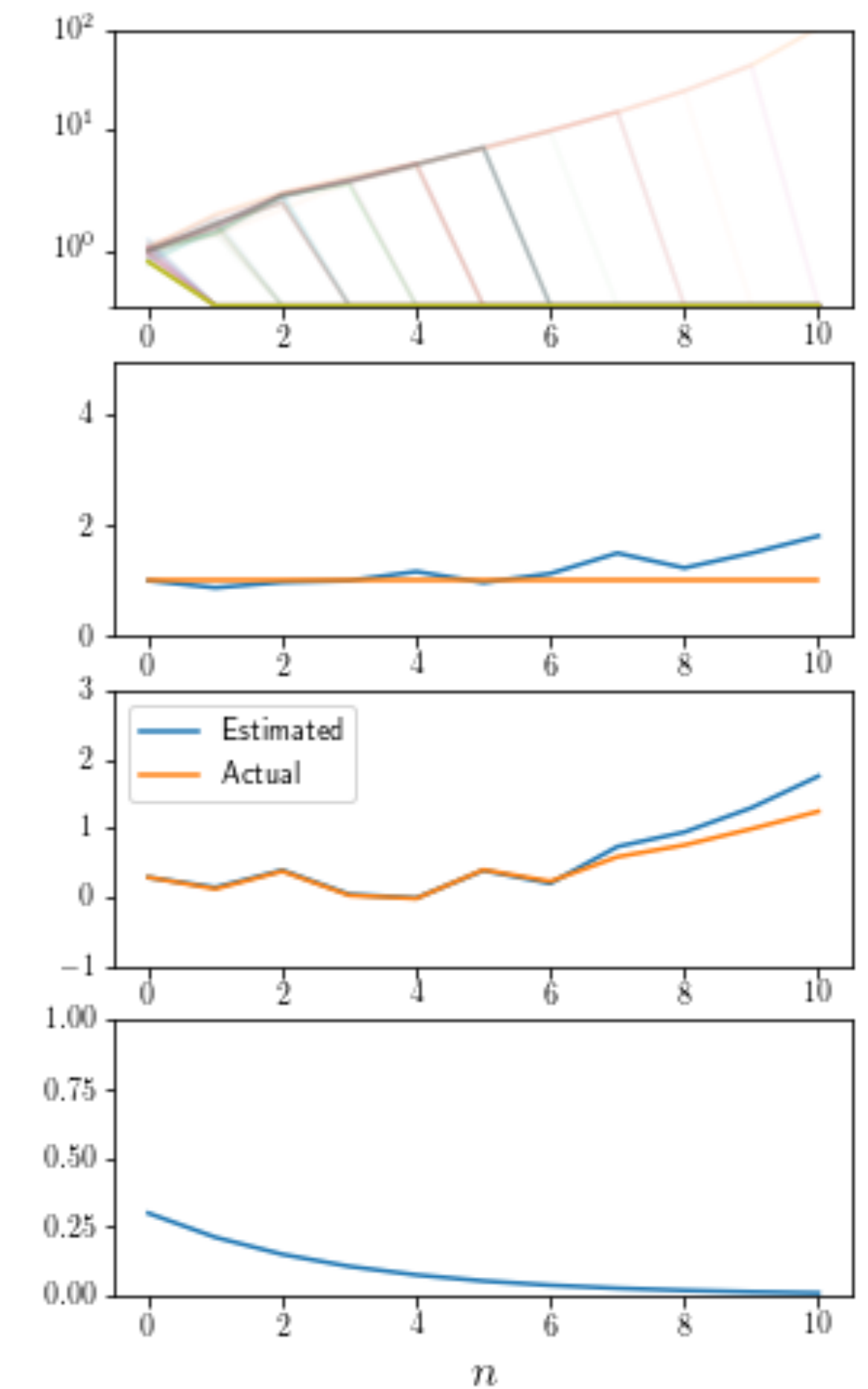
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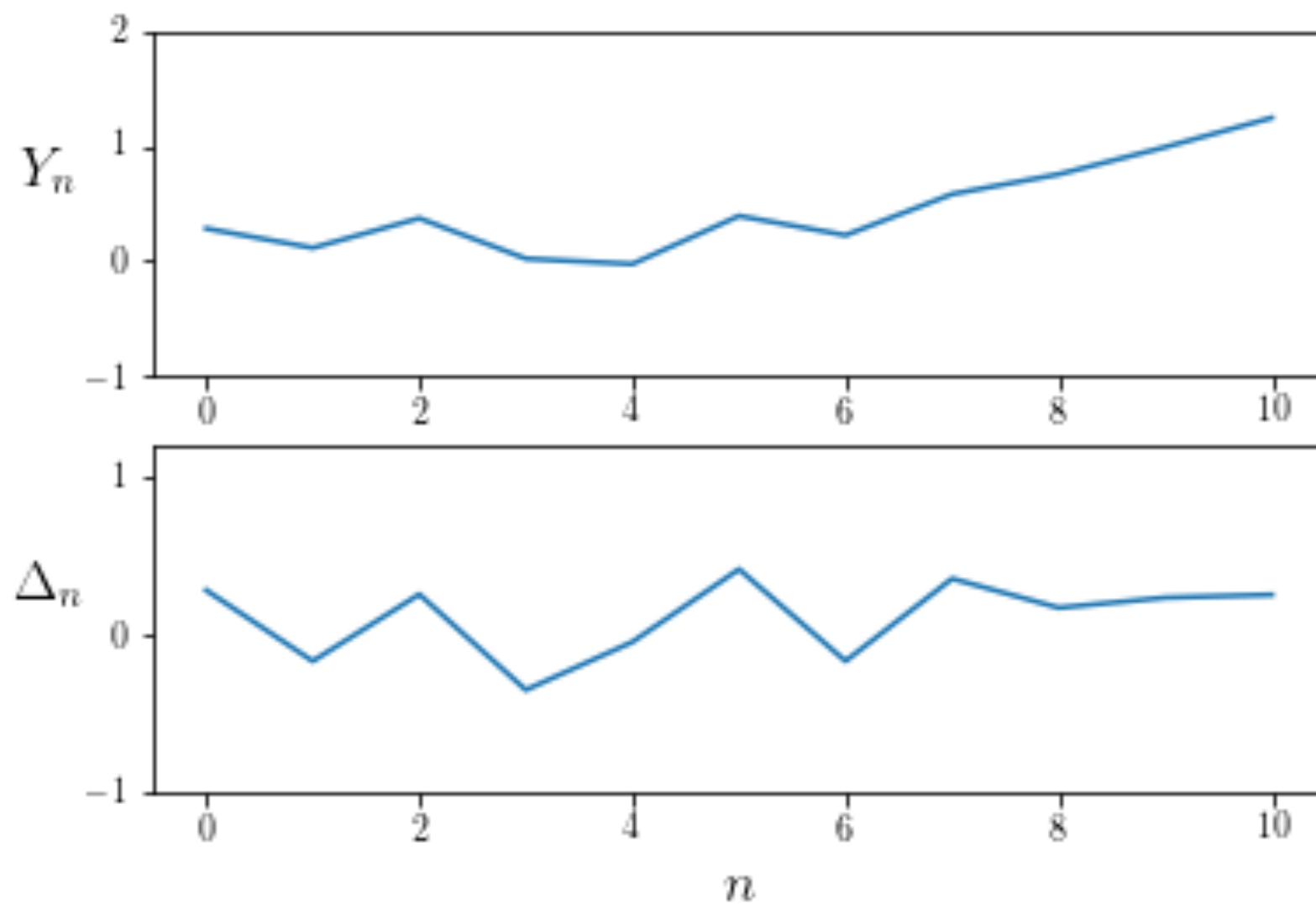
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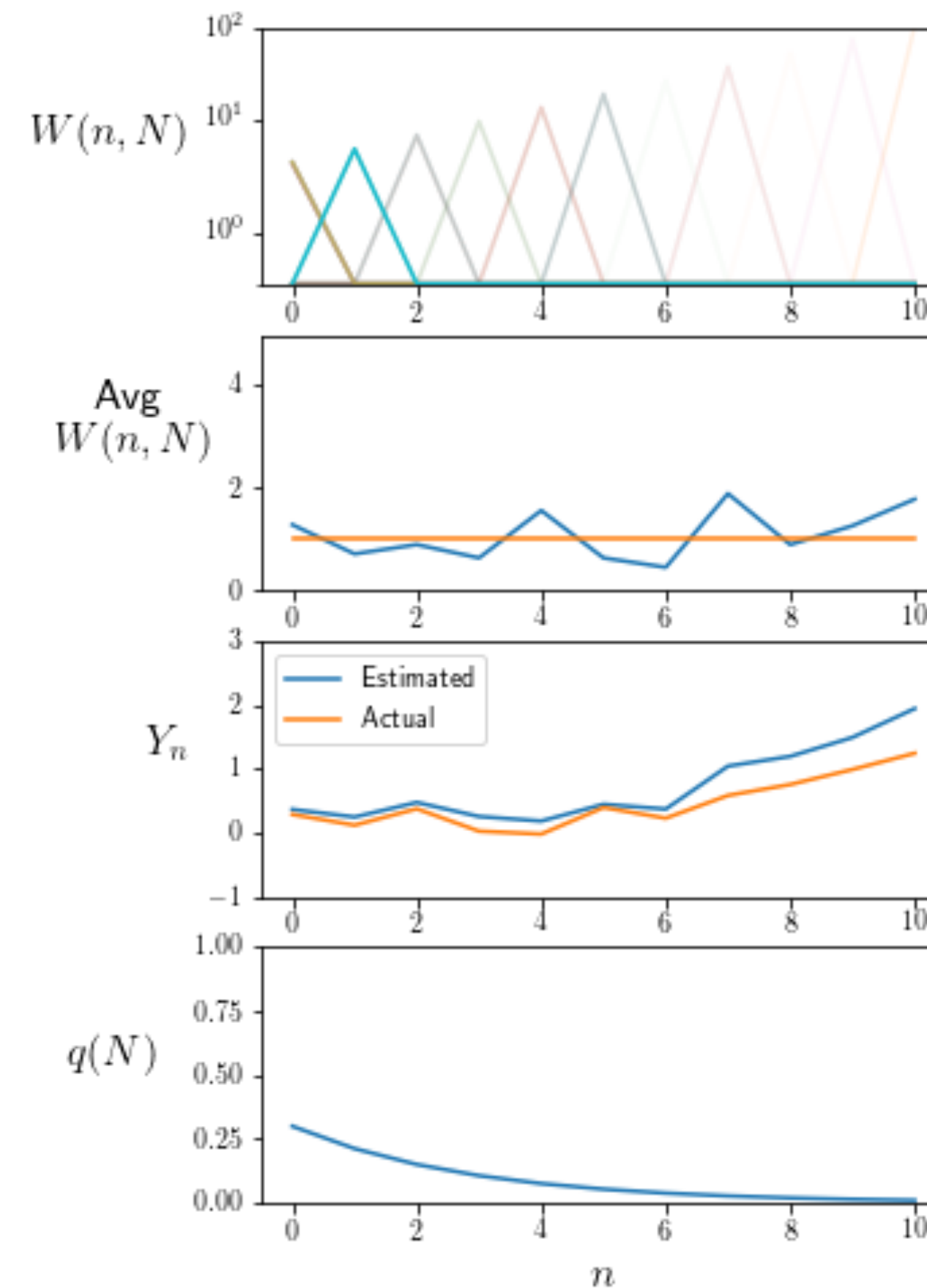
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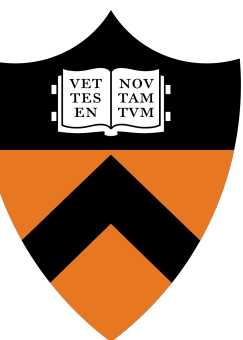
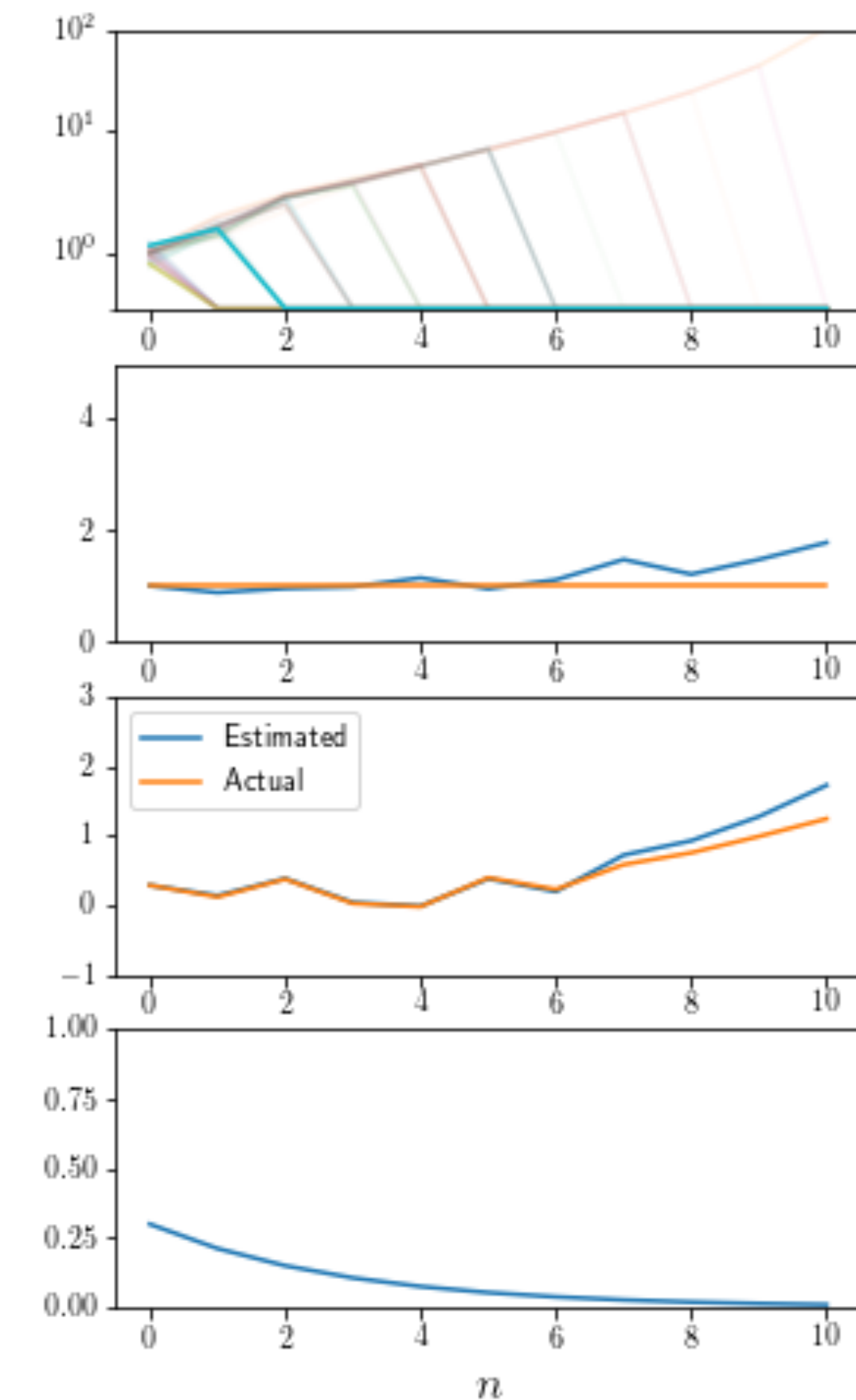
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$$W(n, N) = \frac{1}{q(N)} \mathbb{1}\{n = N\}$$



“Russian roulette”

$$W(n, N) = \frac{1}{1 - \sum_{n'=1}^{n-1} q(n')} \mathbb{1}\{N \geq n\}$$



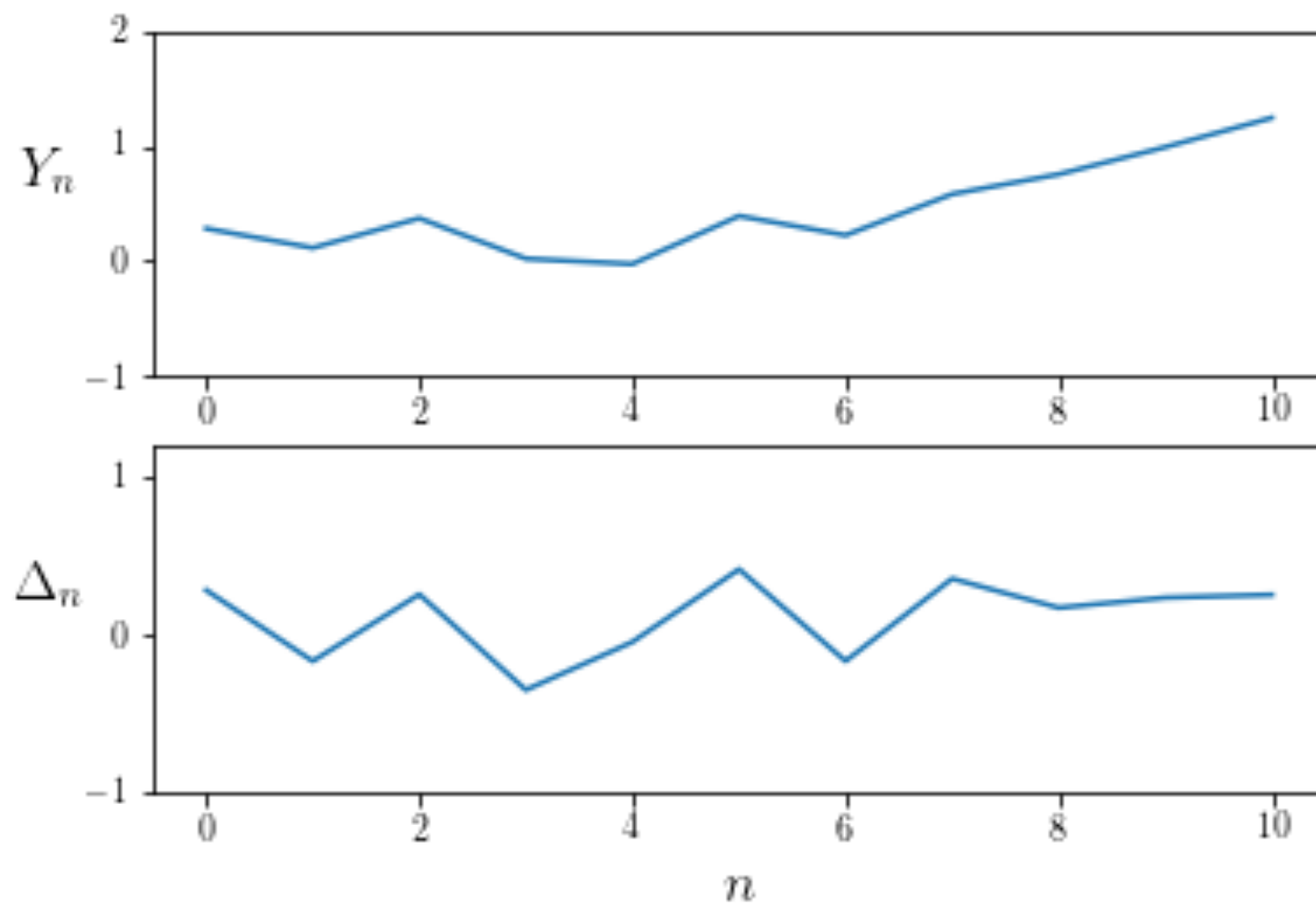
# DEMONSTRATION

General form

$$\hat{Y}_H = \sum_{n=1}^N \Delta_n W(n, N) \quad N \in \{1, \dots, H\} \sim q$$

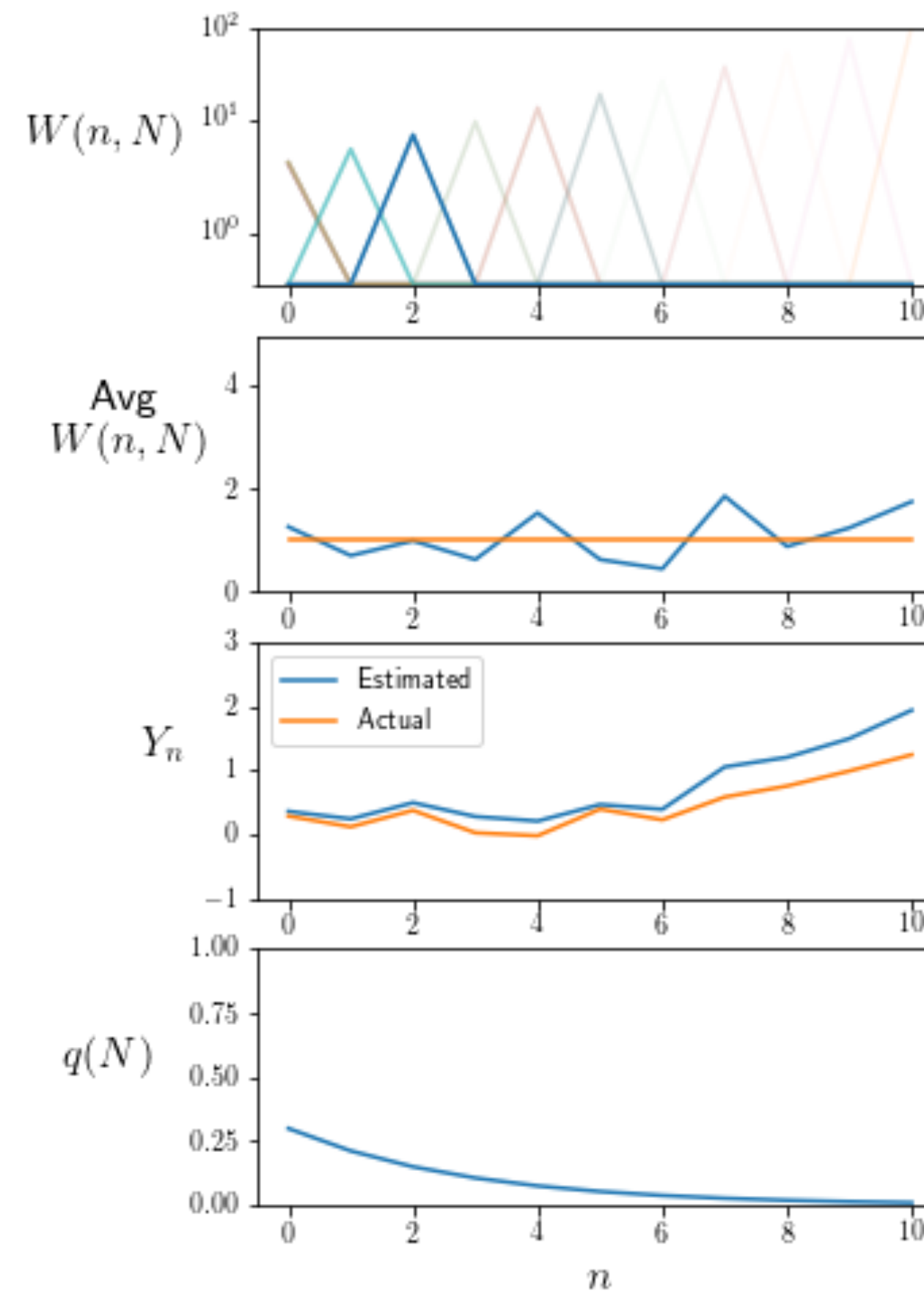
$$\Delta_n = \begin{cases} Y_n - Y_{n-1} & n > 1 \\ Y_1 & n = 1 \end{cases}$$

Ground truth



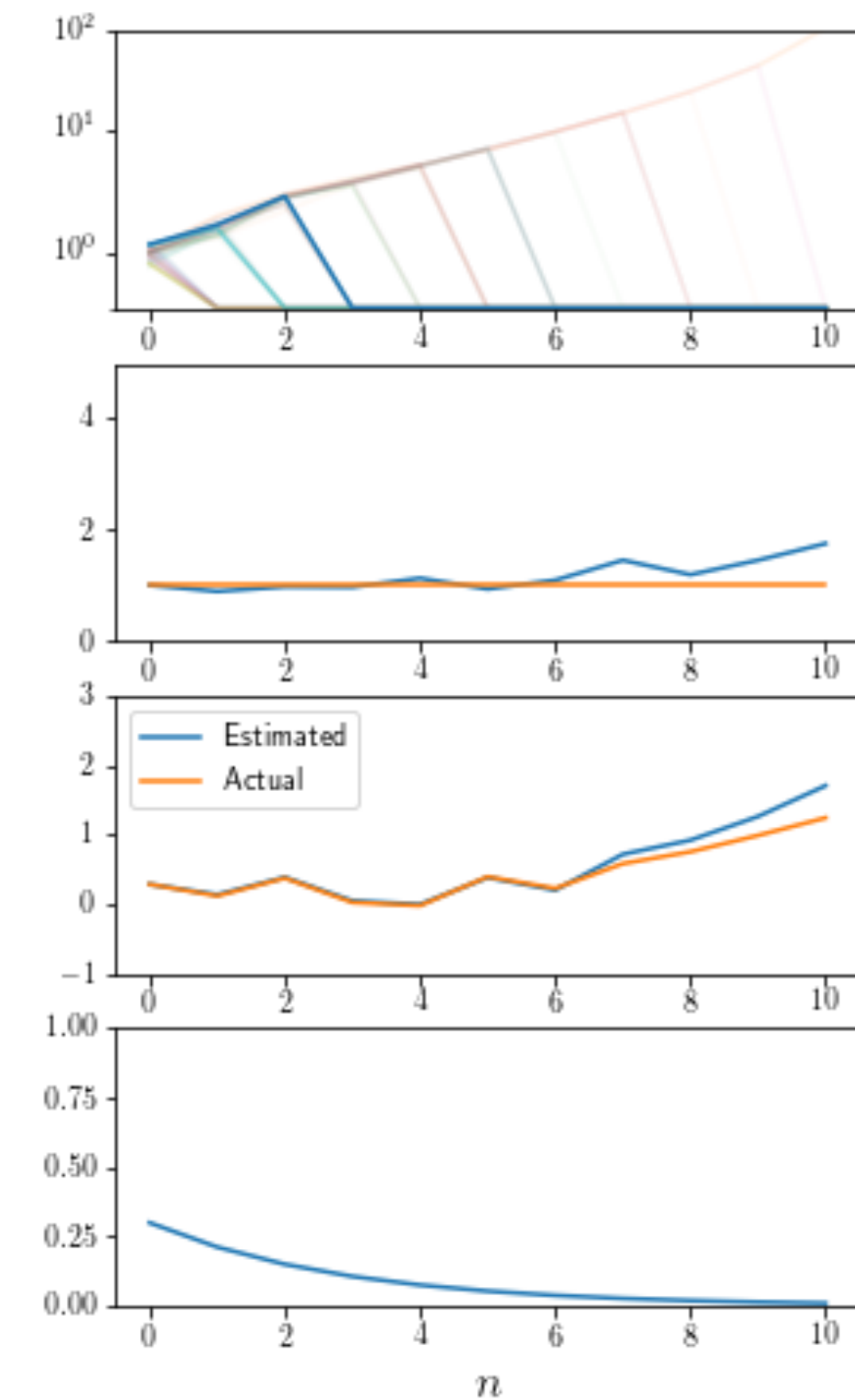
“Single sample”

$$W(n, N) = \frac{1}{q(N)} \mathbb{1}\{n = N\}$$



“Russian roulette”

$$W(n, N) = \frac{1}{1 - \sum_{n'=1}^{n-1} q(n')} \mathbb{1}\{N \geq n\}$$



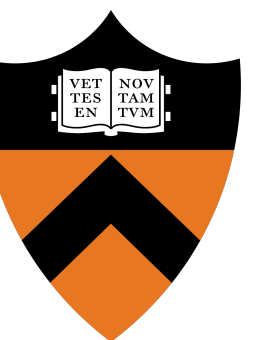


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# RANDOMIZED TELESCOPES FOR OPTIMIZATION

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- Randomized Telescopes for optimization = SGD for limits
- Can achieve finite variance and compute for any geometrically converging sequence, or sufficiently fast polynomially converging sequences ( $p > 3/2$ ).
- This means we can optimize the limit itself rather than an approximation, with provable convergence rates and anytime guarantees!

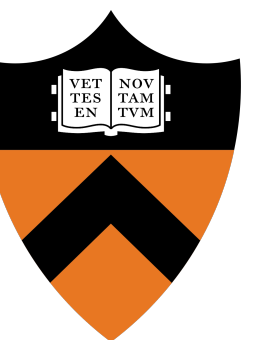


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# PRACTICAL RECIPE

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- Pick a (large) maximal truncation
- Estimate the convergence properties of  $\Delta_n$  online
- Adapt sampling probabilities and learning rate to balance computation and variance, and maximize a lower bound on increase in optimization efficiency relative to maximal truncation



# EXPERIMENTS

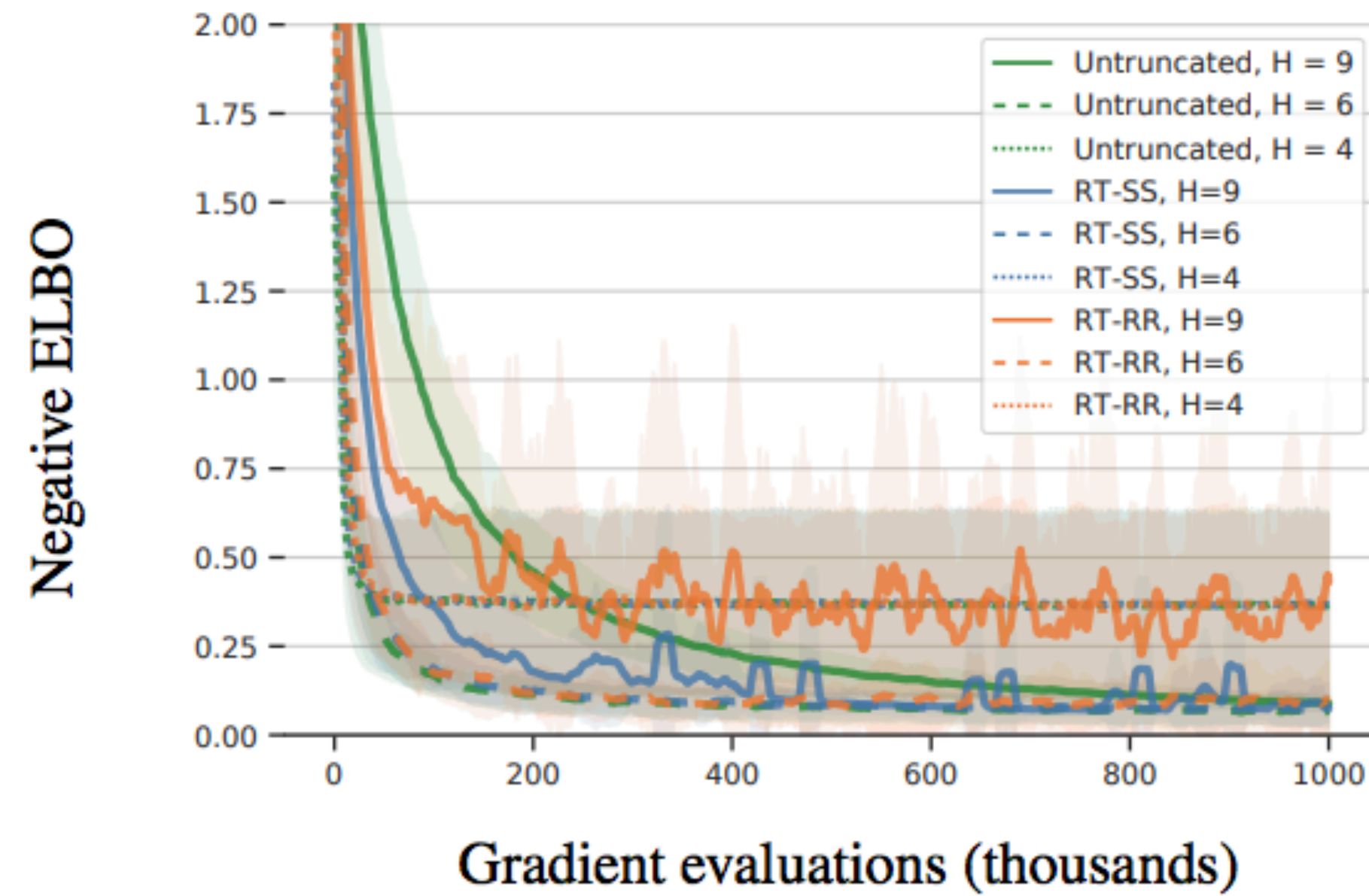


Figure 1. Lotka-Volterra parameter inference

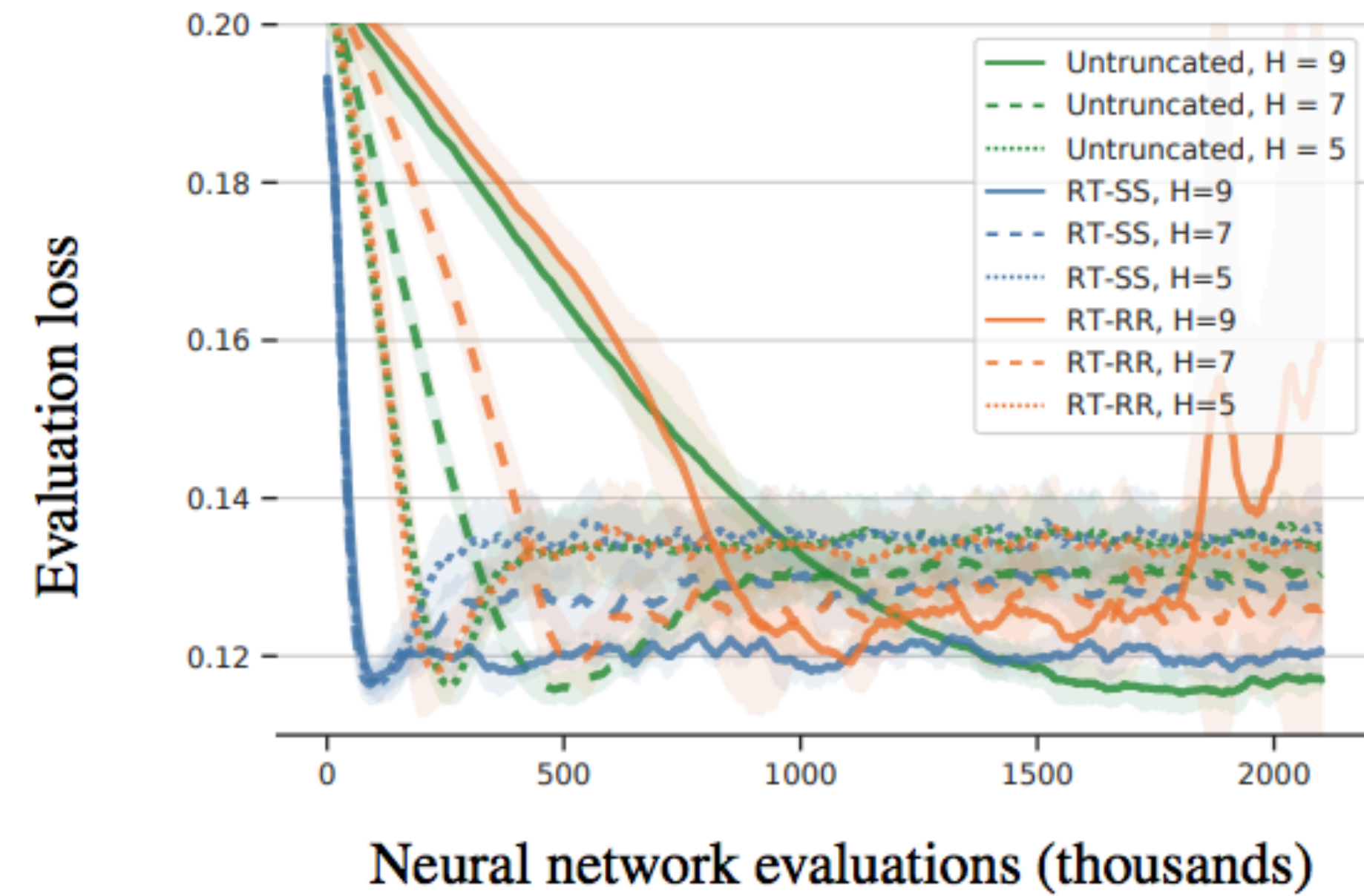
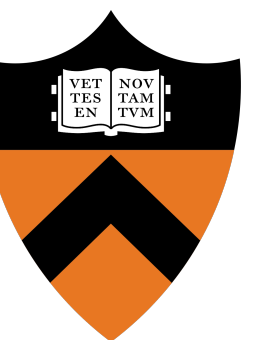
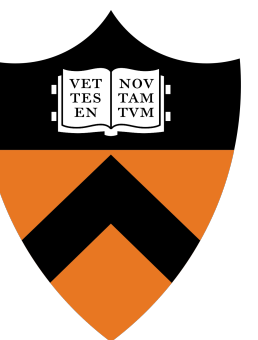


Figure 2. MNIST learning rate meta-optimization



# LIMITATIONS AND EXTENSIONS

- Does not accelerate very high-dimensional problems (e.g., optimizing an RNN): our model of  $\Delta_n$  suffers in high dimensions and adaptive sampling falls back on the maximal truncation
- Only support SGD: possible extensions to Adam, quasi-Newton, ...
- Use series acceleration or predictive models to accelerate convergence to the limit





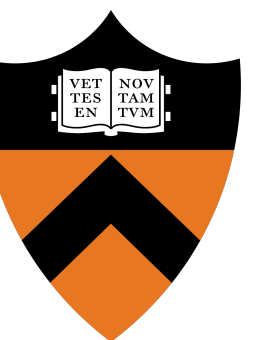
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# Neural Model-Order Reduction

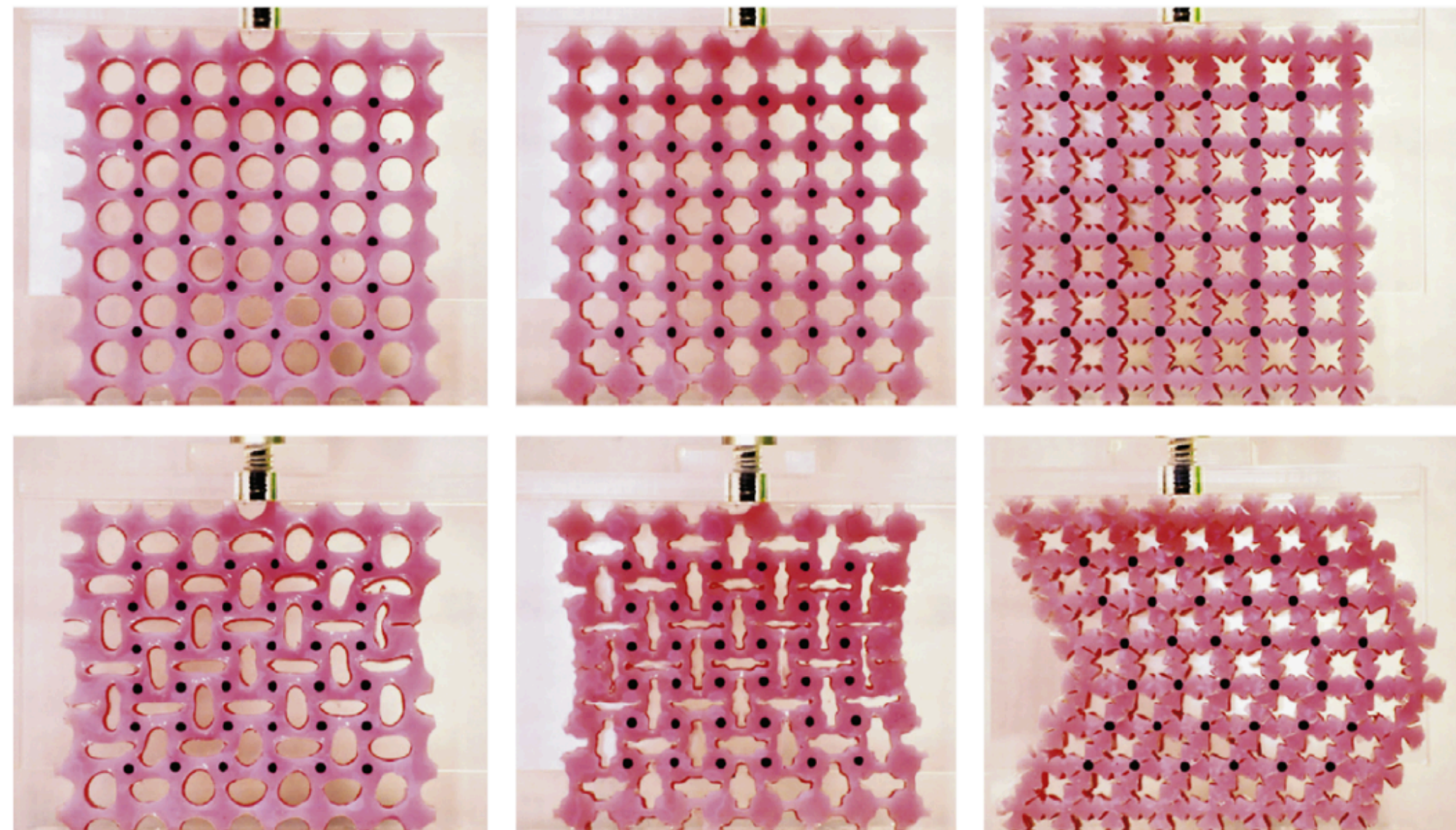
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with Tianju Xie, Jordan Ash, Geoffrey Roeder, Ryan P. Adams

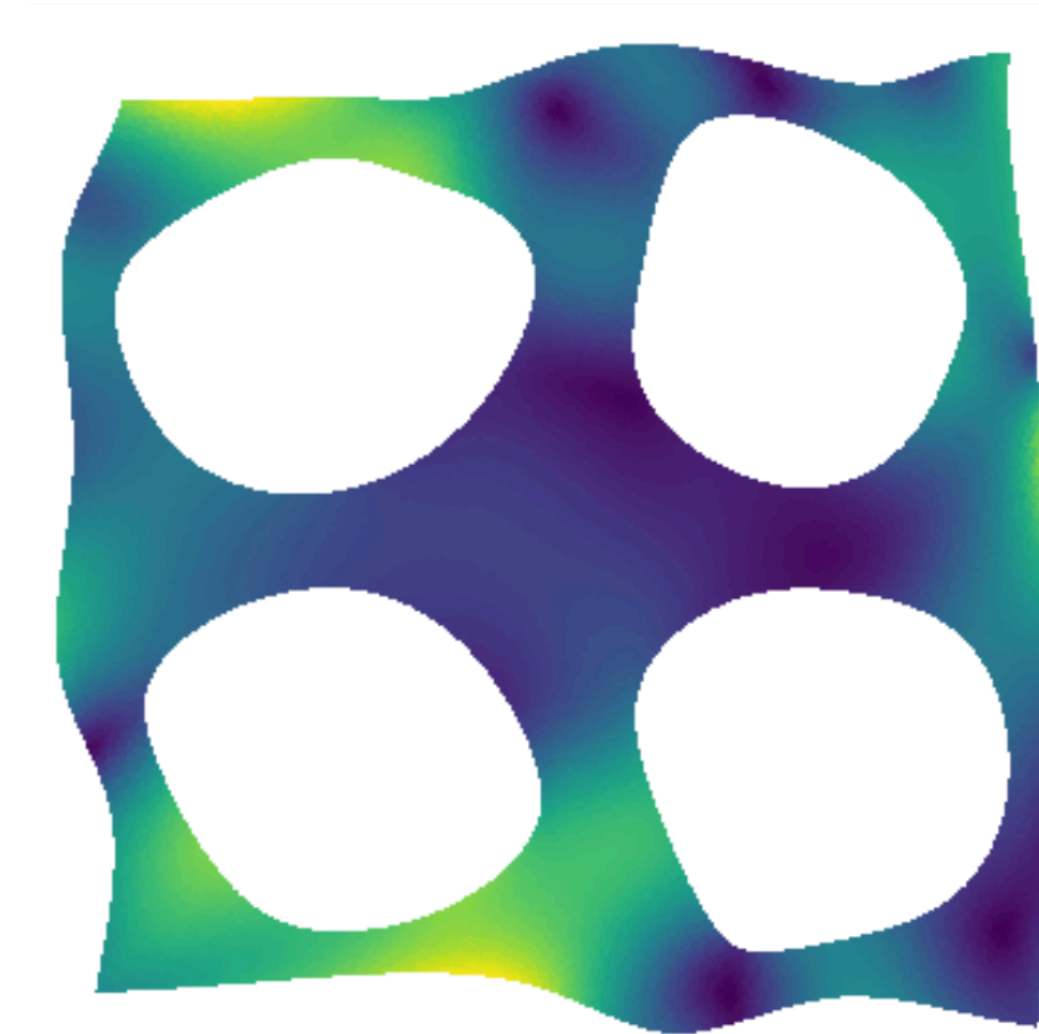
In progress



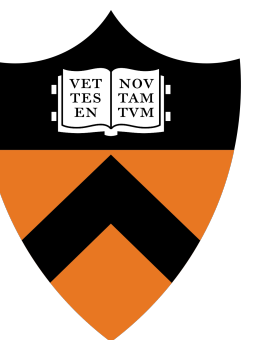
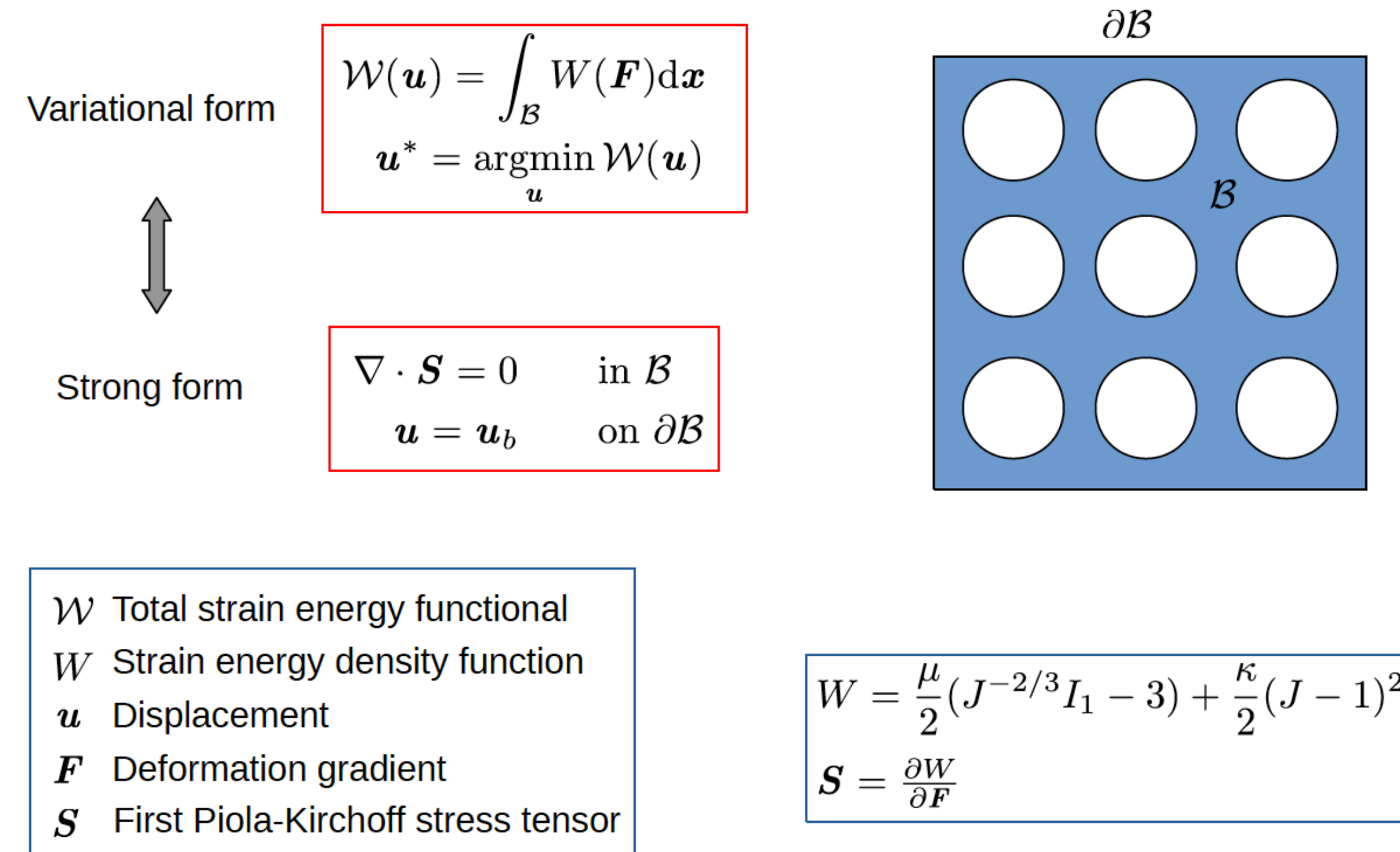
# NEURAL MODEL-ORDER REDUCTION



Overvelde & Bertoldi, 2014

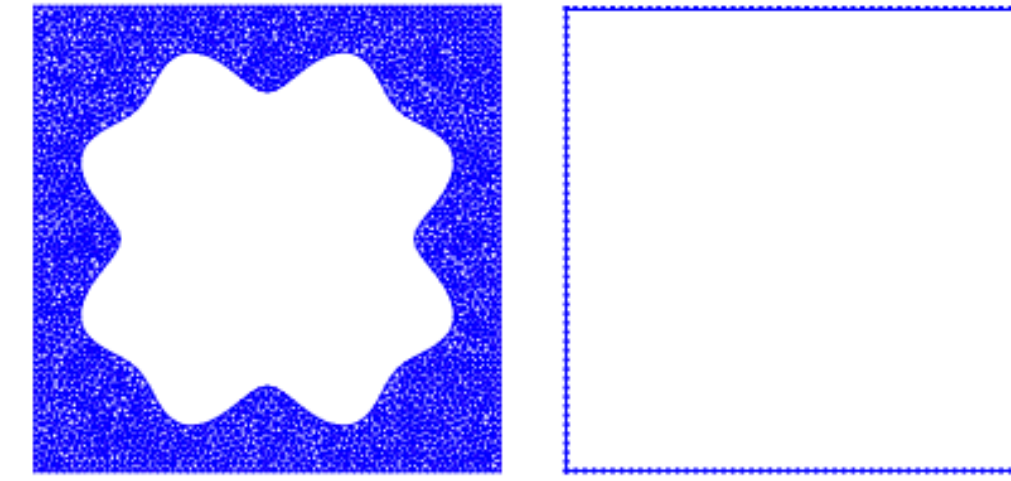
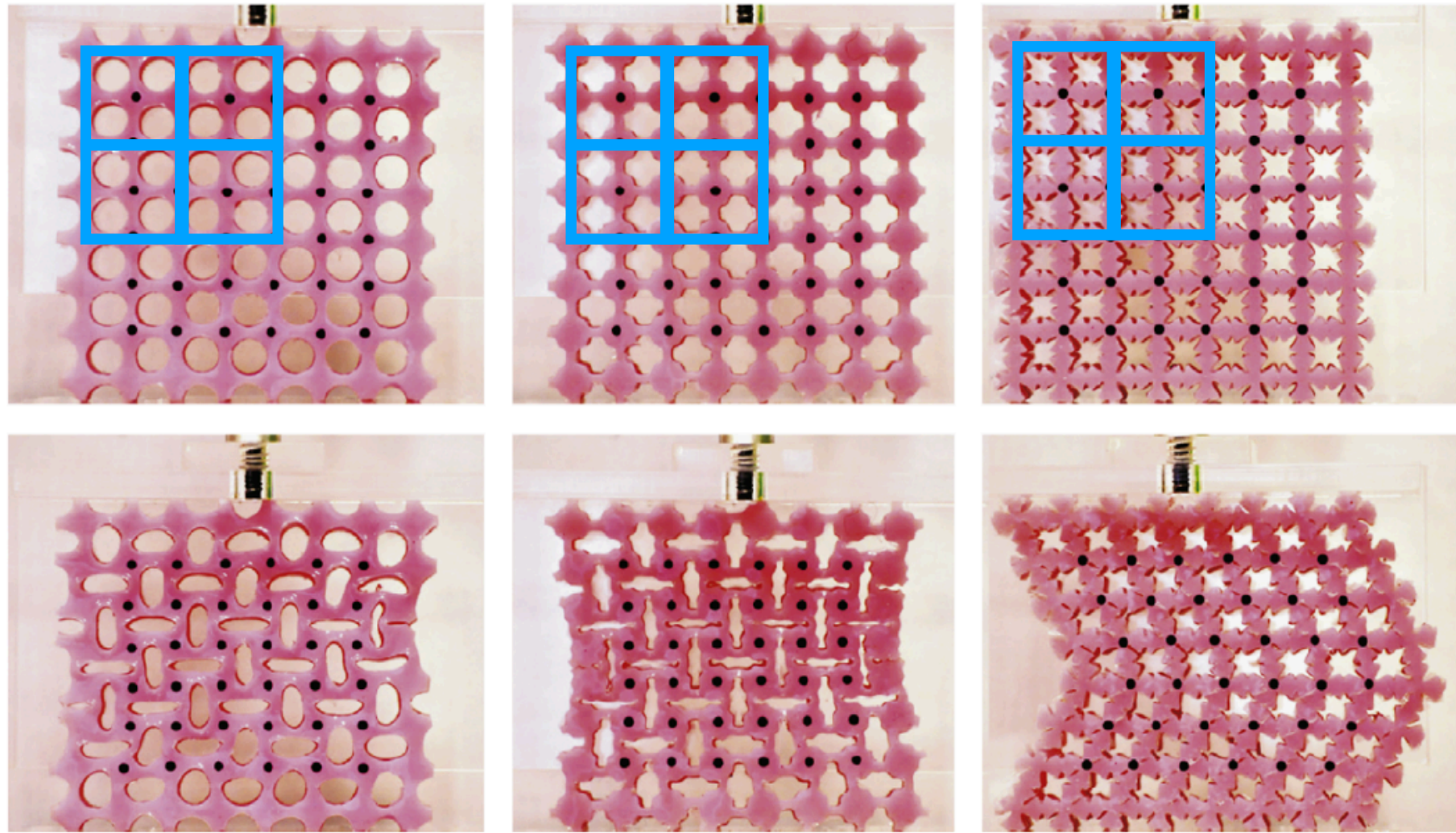


# NEURAL MODEL-ORDER REDUCTION



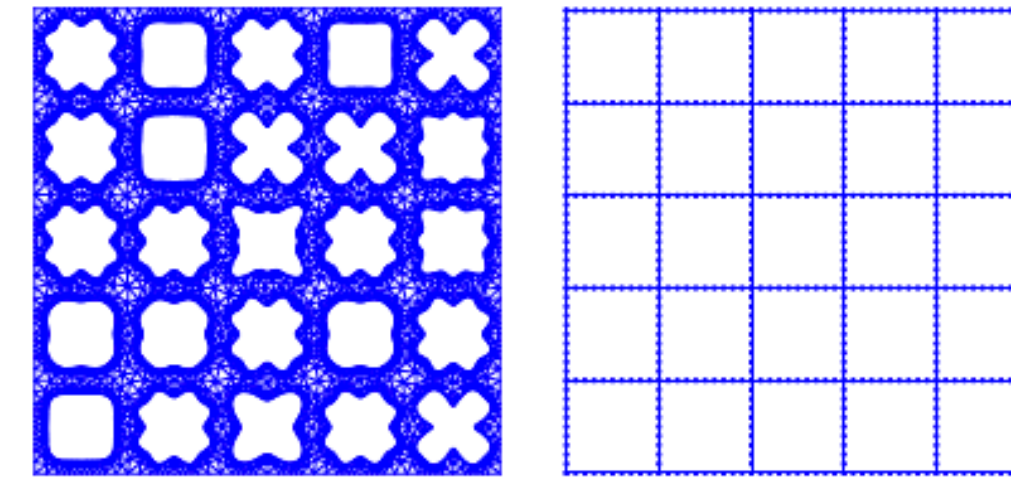


# NEURAL MODEL-ORDER REDUCTION



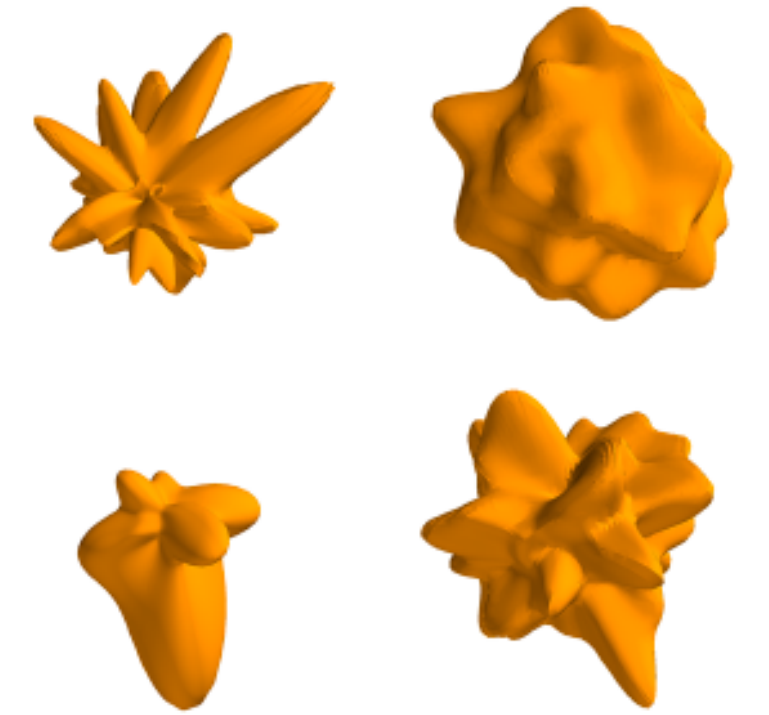
(a) Full order

(b) Reduced order



(c) Full order

(d) Reduced order



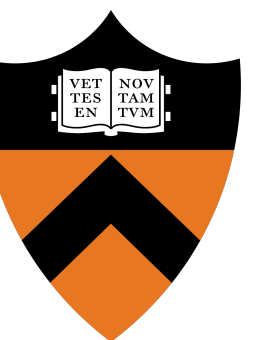
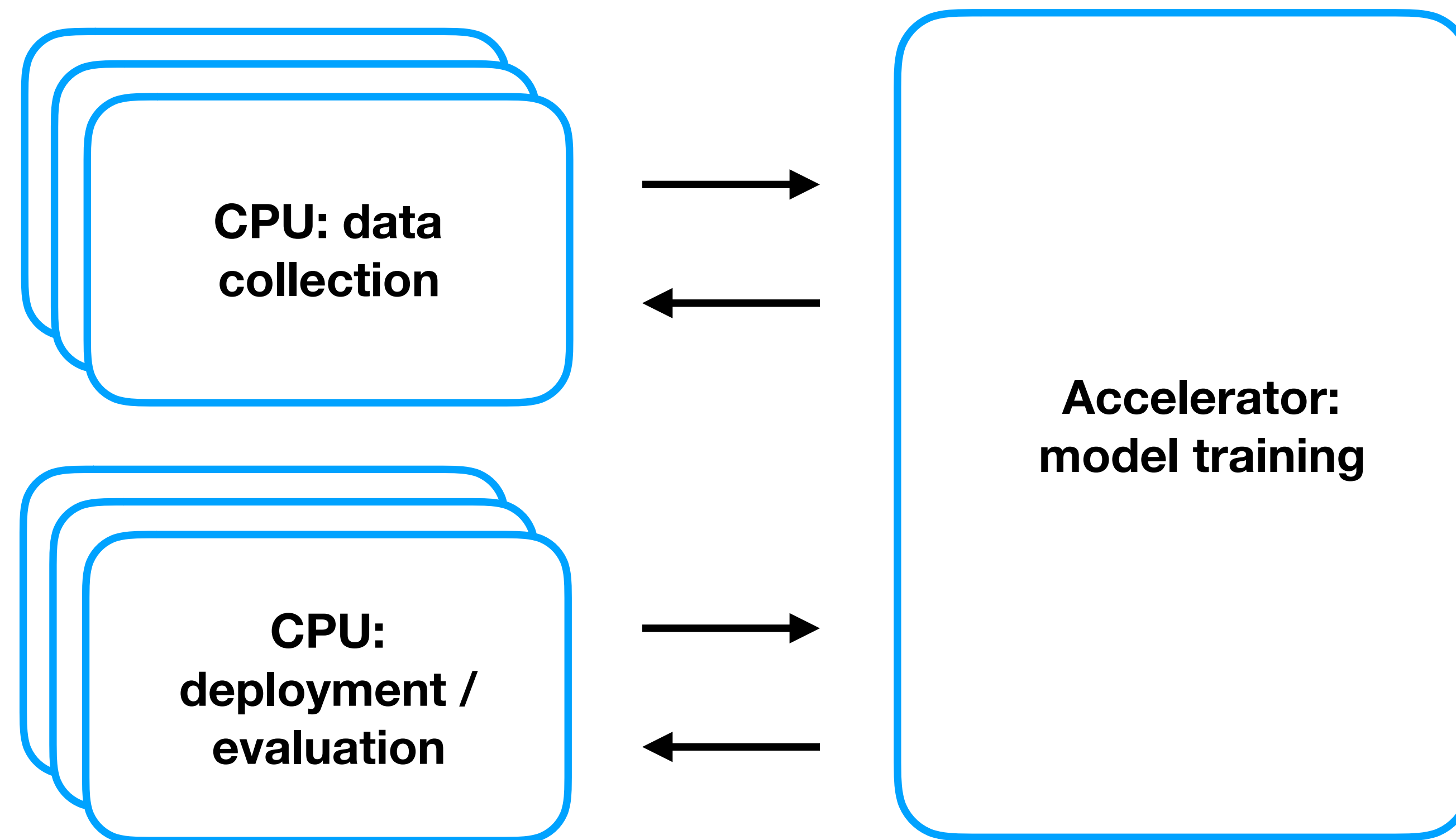
3-D pore shapes from Gaussian process priors.

$$\mathcal{W}(\mathbf{u}) = \int_{\mathcal{B}} W(\mathbf{F}) d\mathbf{x} = \sum_{c \in \mathcal{B}} \int_c W(\mathbf{F}) d\mathbf{x}$$

$$\min \mathcal{W}(\mathbf{u}) = \min_{\mathbf{u}^{\delta c}} \sum_c \min_{\mathbf{u}^c} \mathcal{W}^c(\mathbf{u}^c)$$



# NEURAL MODEL-ORDER REDUCTION

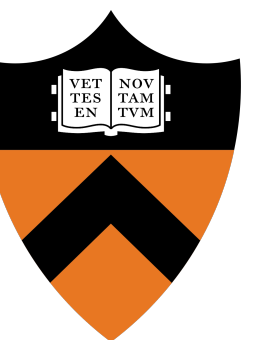


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# NEURAL MODEL-ORDER REDUCTION

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- Model energy in cell as function of boundary deformation
- Collect data with small, cheap simulations to train neural network
- Use to efficiently solve large systems and optimize pores
- Tricks: train on energy **derivatives** (stress-strain relations) as well as values; exploit invariances with polar coordinates + convolution; use linear elastic model for regularization / prior



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# THANKS!

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