

# Understanding Regression-adjusted Control Variate

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Sobolev embedding and rare event

**Joint work with** Jose Blanchet, Haoxuan Chen, Lexing Ying

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<https://2prime.github.io/>

# ML Nowadays

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“entertainment, advising”

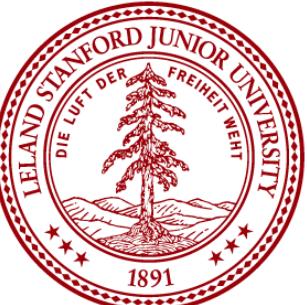


**Midjourney**



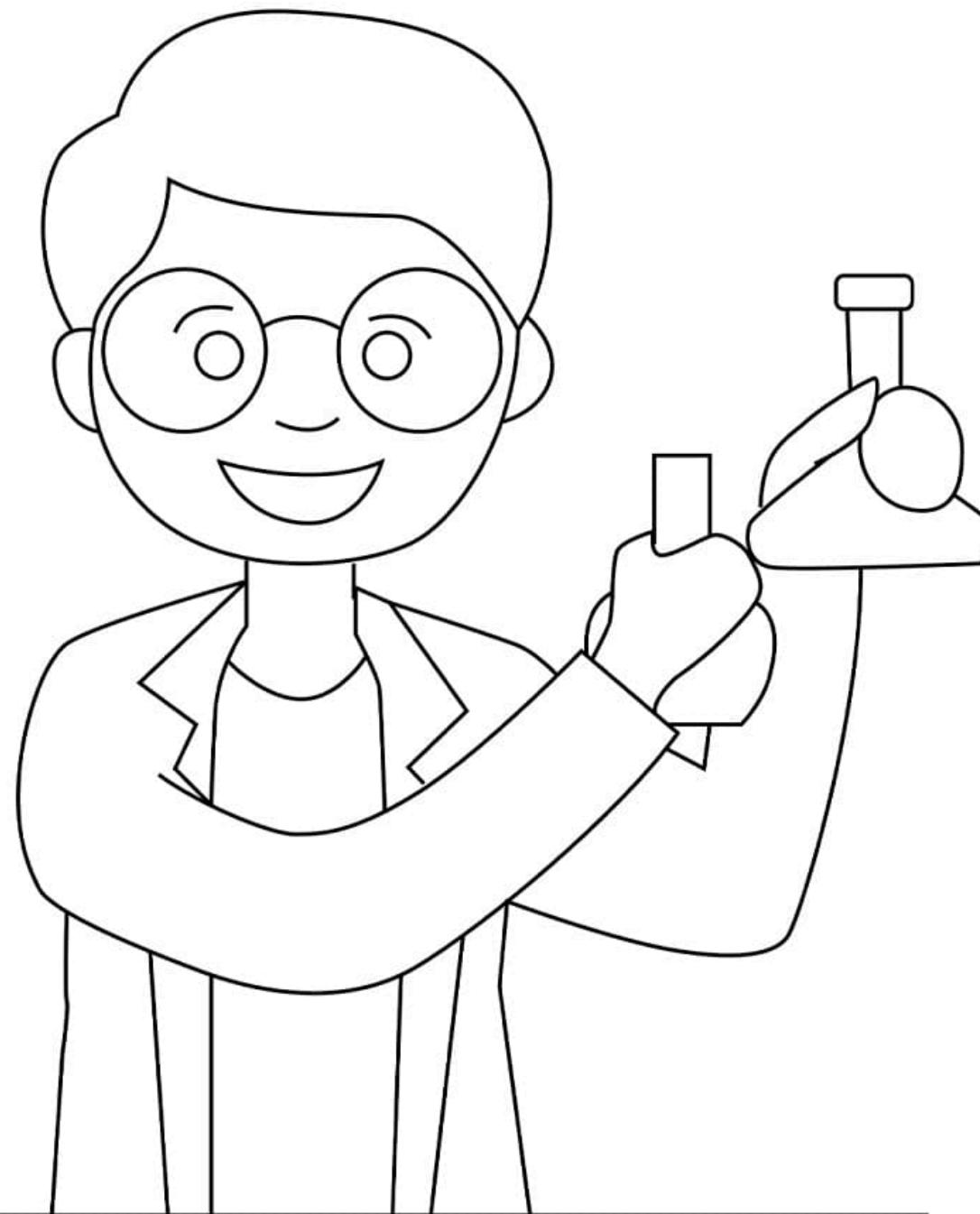
OpenAI  
ChatGPT **4.0**

**《science》**

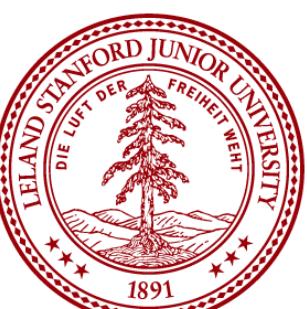


# We want Guarantee!

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**Theorem** If you randomly collect  
( ) data, then you can achieve  
( ) accuracy with your AI!



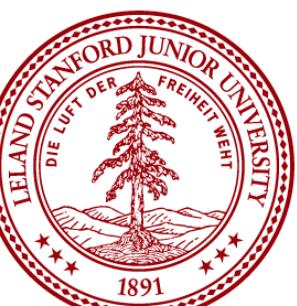
# We want Guarantee!

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**Theorem** If you randomly collect  
( ) data, then you can achieve  
( ) accuracy with your AI!

**Assumption 1.** Xxx  
**Assumption 2.** Xxx  
**Assumption 3.** Xxx  
**Assumption 4.** Xxx



# ML for Science nowadays

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# Debiasing ML for Science

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You can prove theorem, but I still don't trust you!

Can we debias ML estimator or use it in an unbiased way?

# Debiasing ML for Science

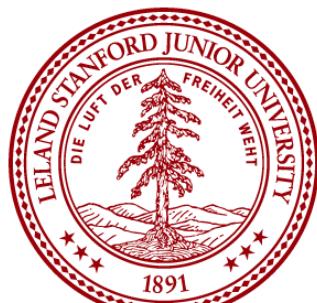
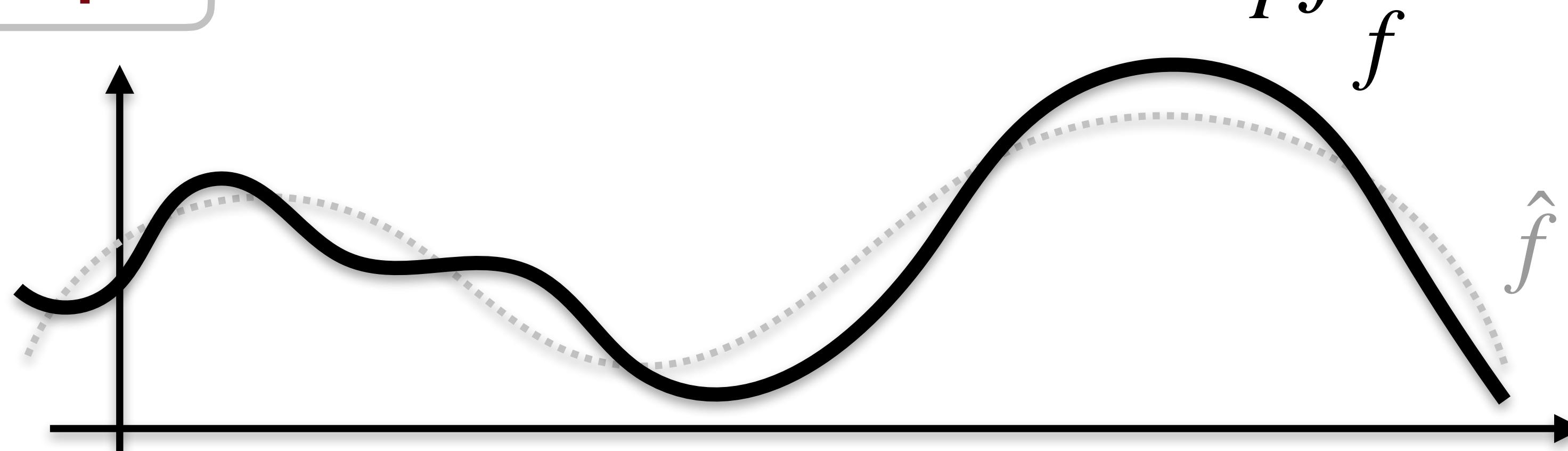
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Can we debias ML estimator or use it in an unbiased way?

## Example

Monte Carlo Estimate  $\mathbb{E}_P f$



# Debiasing ML for Science

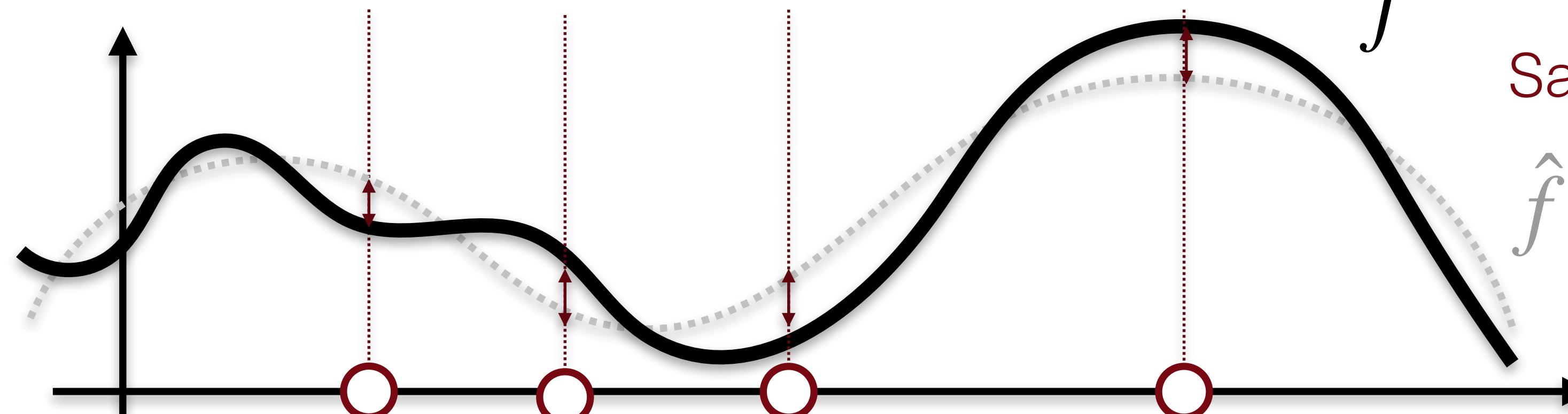
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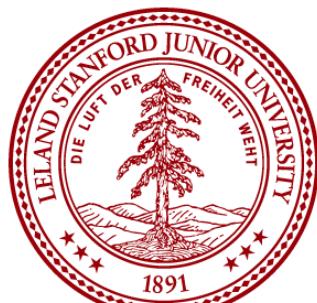
Can we debias ML estimator or use it in an unbiased way?

## Example

Monte Carlo Estimate  $\mathbb{E}_P f$



Sample extra data to know  $f - \hat{f}$



# Debiasing ML for Science

You can prove theorem, but I still don't trust you!



*“Regression-adjusted control variate”*

Can we debias ML estimator or use it in an unbiased way?

## Example

Monte Carlo Estimate  $\mathbb{E}_P f$

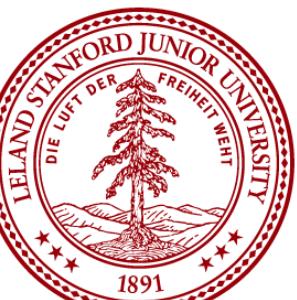
### Step 1

Using half of the data to estimate  $\hat{f}$

### Step 2

$$\mathbb{E}_P f = \mathbb{E}_P(\hat{f}) + \mathbb{E}_P(f - \hat{f})$$

Low order term



# “Modern” regression-adjusted cv

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Trace estimation:

Hutch++ Lin 17 Numerische Mathematik Mewyer-Musco-Musco-Woodruff 20

Dimension Reduction:

Sobczyk and Luisier Neurips 22

Conformal Prediction:

Conformalized quantile regression Romano-Patterson-Candes Neurips 19

Gradient Estimation

Shi-Zhou-Hwang-Tisias-Mackey Neurips 22 outstanding paper

Causal Inference:

Double Robust estimation ....



# Debiasing ML for Science



Is this algorithm statistical optimal?

When this improves MC estimator?

Can we debias ML estimator or use it in an unbiased way?

## Example

Monte Carlo Estimate  $\mathbb{E}_P f$

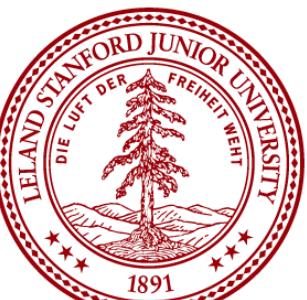
### Step 1

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$$\mathbb{E}_P f = \mathbb{E}_P(\hat{f}) + \mathbb{E}_P(f - \hat{f})$$

Low order term



# Understanding this statistically...



Is this algorithm statistical optimal?

Why consider  $q$ -th moment?

When this improves MC estimator?

Can we debias ML estimator or use it in an unbiased way?

## Example

Monte Carlo Estimate  $\mathbb{E}_P f$   $\mathbb{E}_P f^q, f \in W^{s,p}$

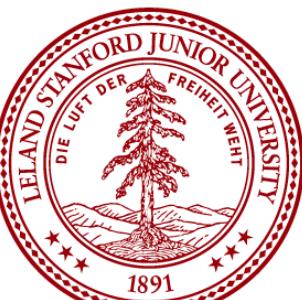
## Step 1

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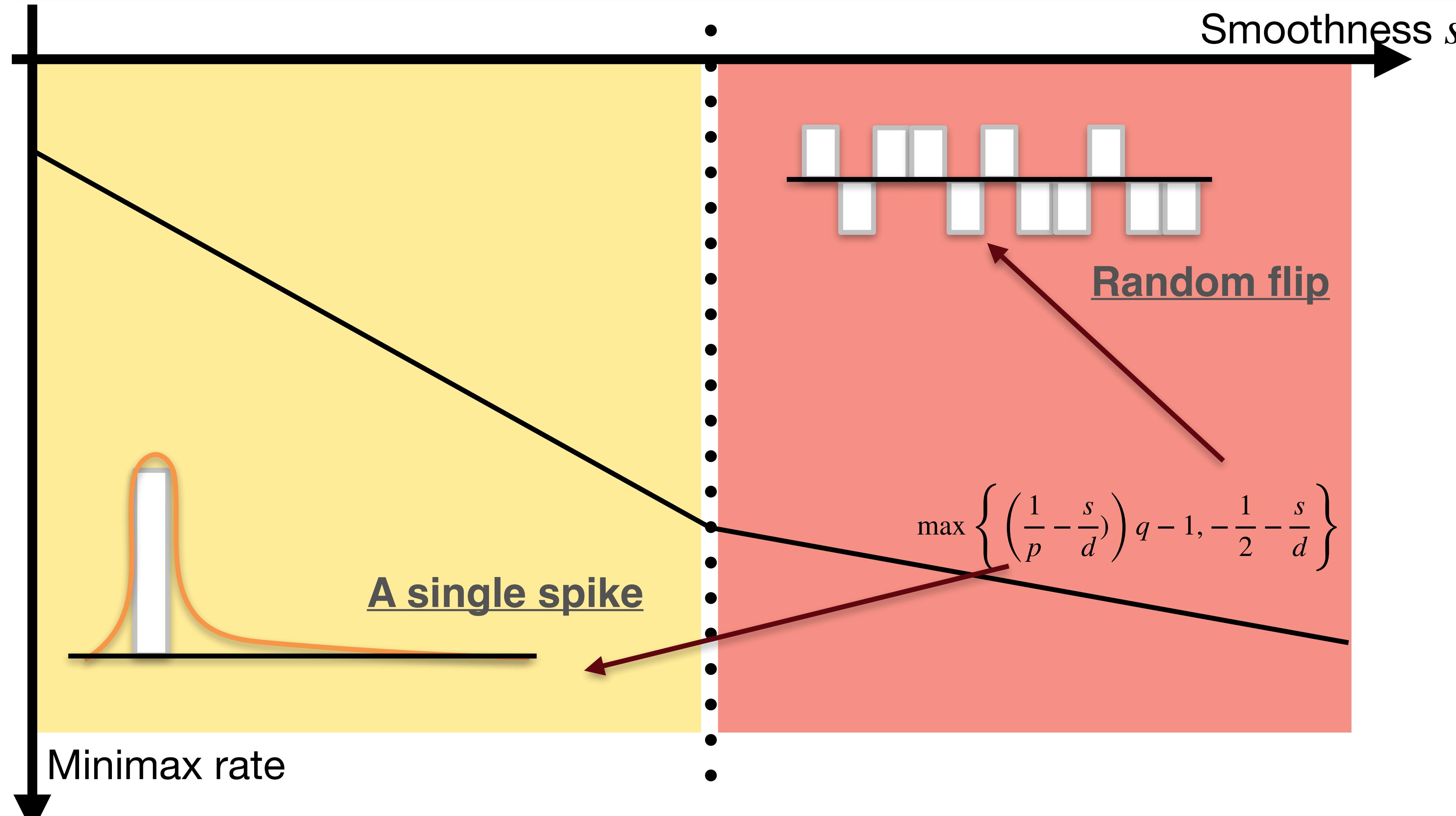
## Step 2

$$\mathbb{E}_P f^q = \mathbb{E}_P (\hat{f})^q + \mathbb{E}_P (f - \hat{f})^q$$

Low order term

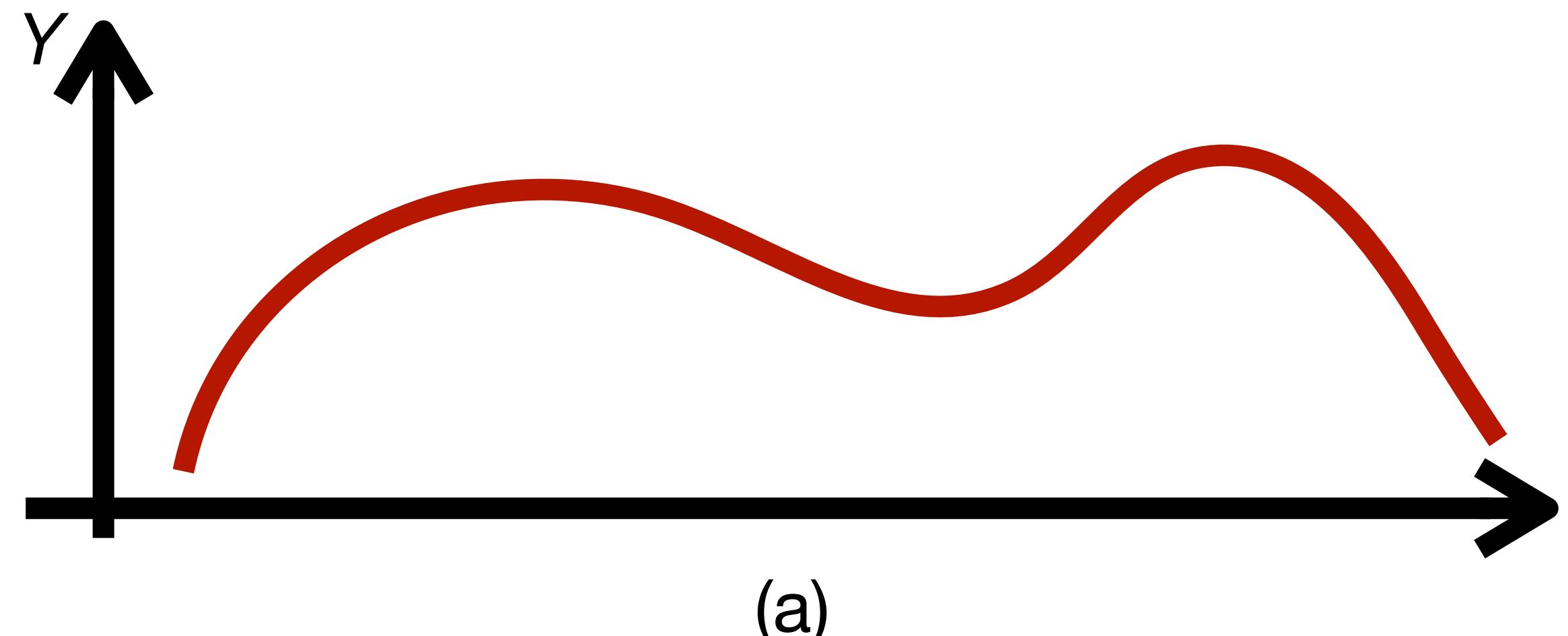


# Setting the information theoretical limit

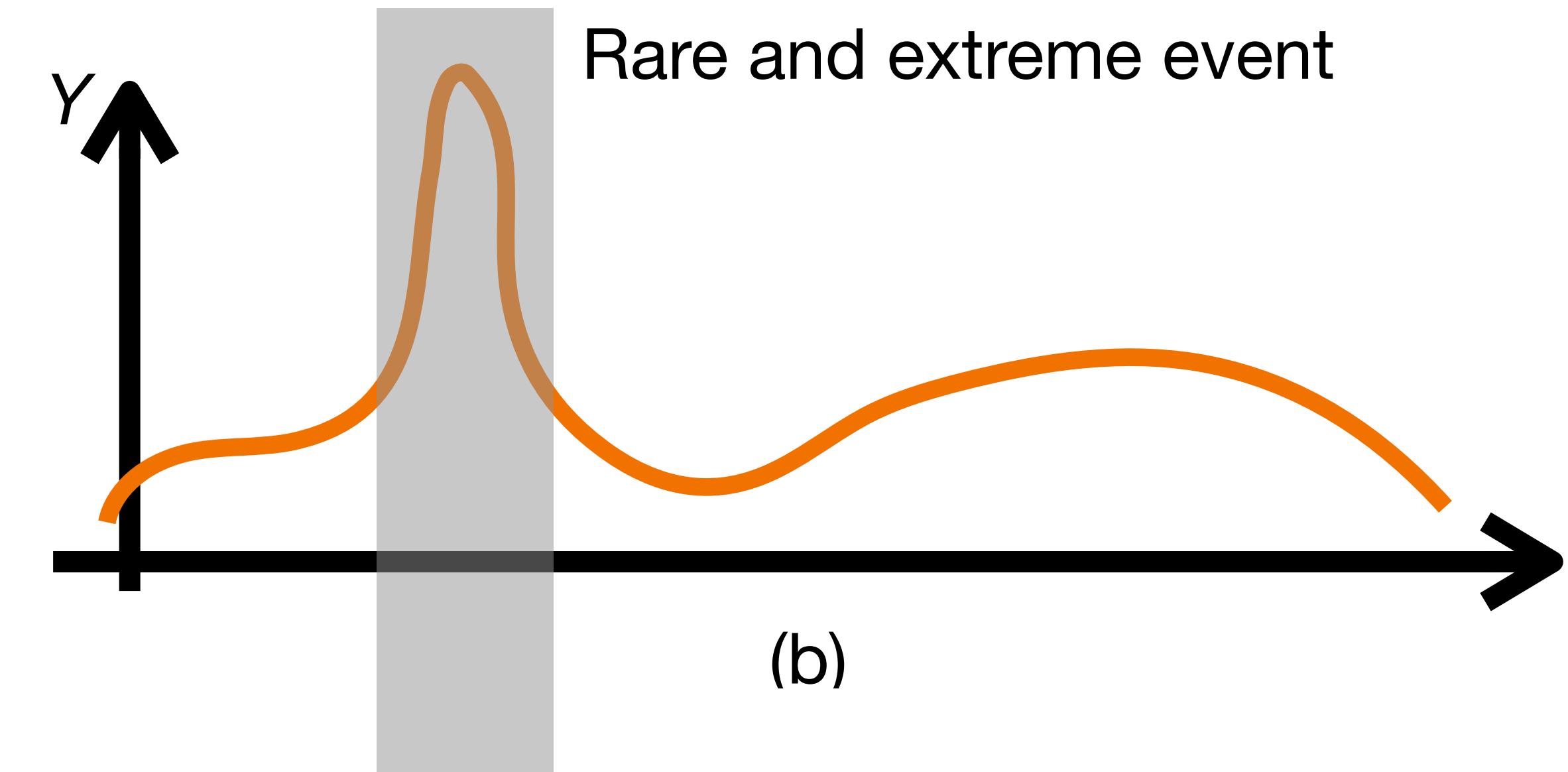


# Rare Event and Smoothness...

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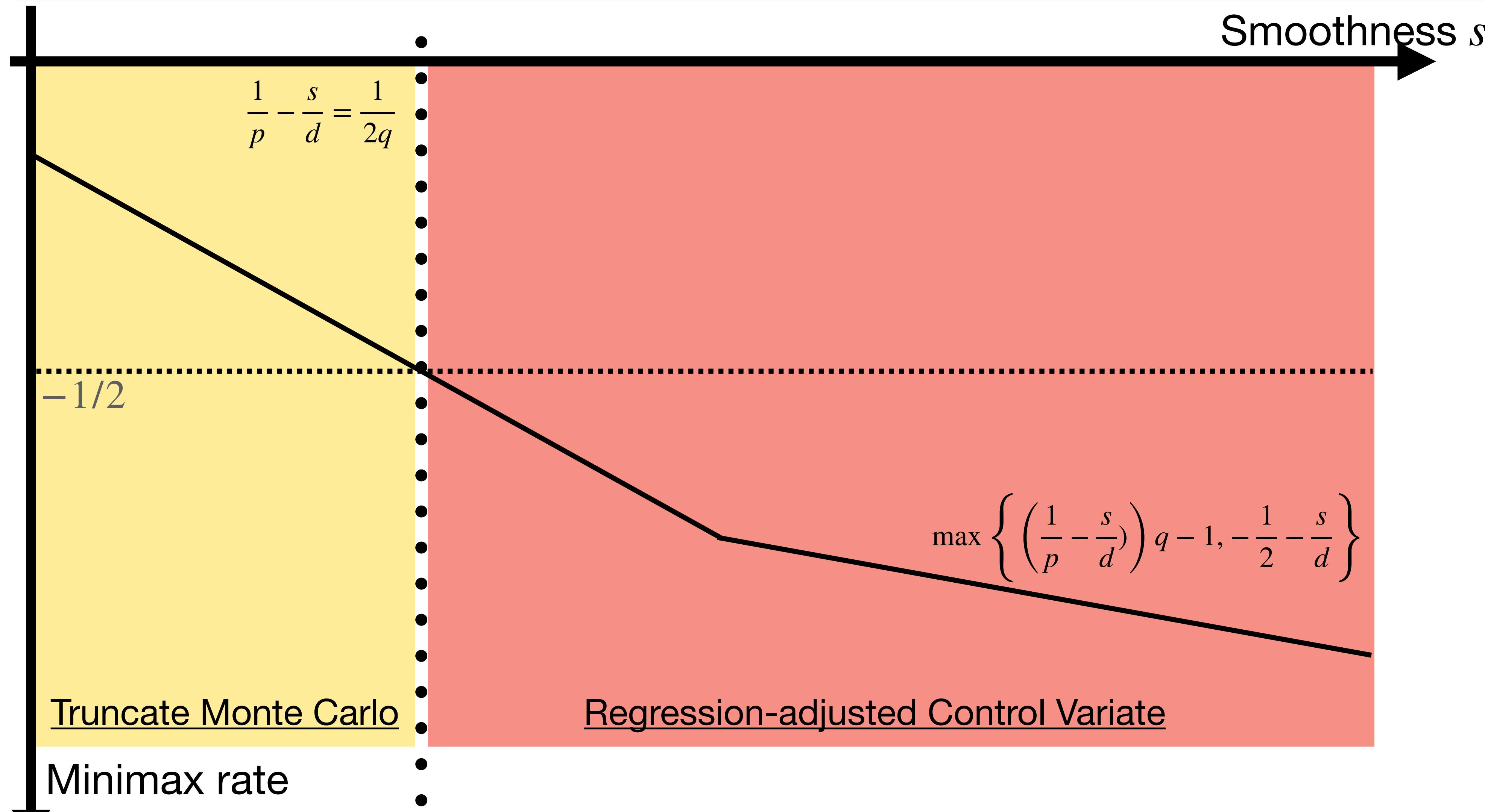
(a)



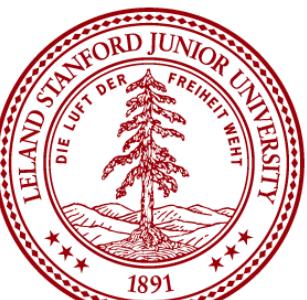
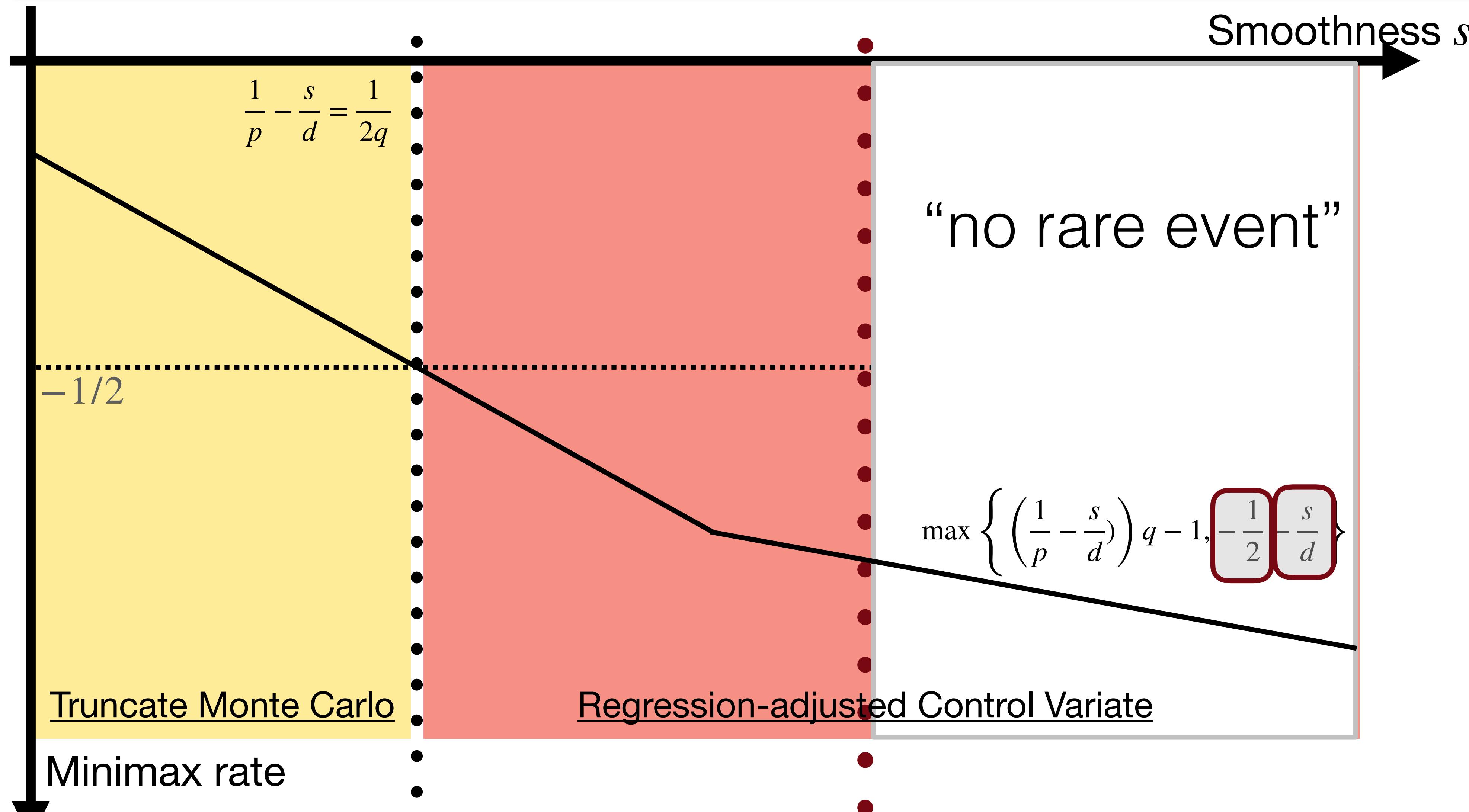
(b)

Rare and extreme event

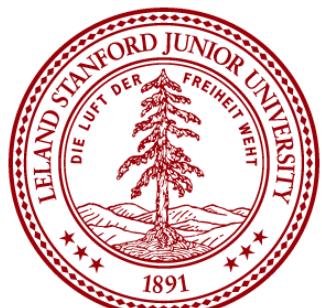
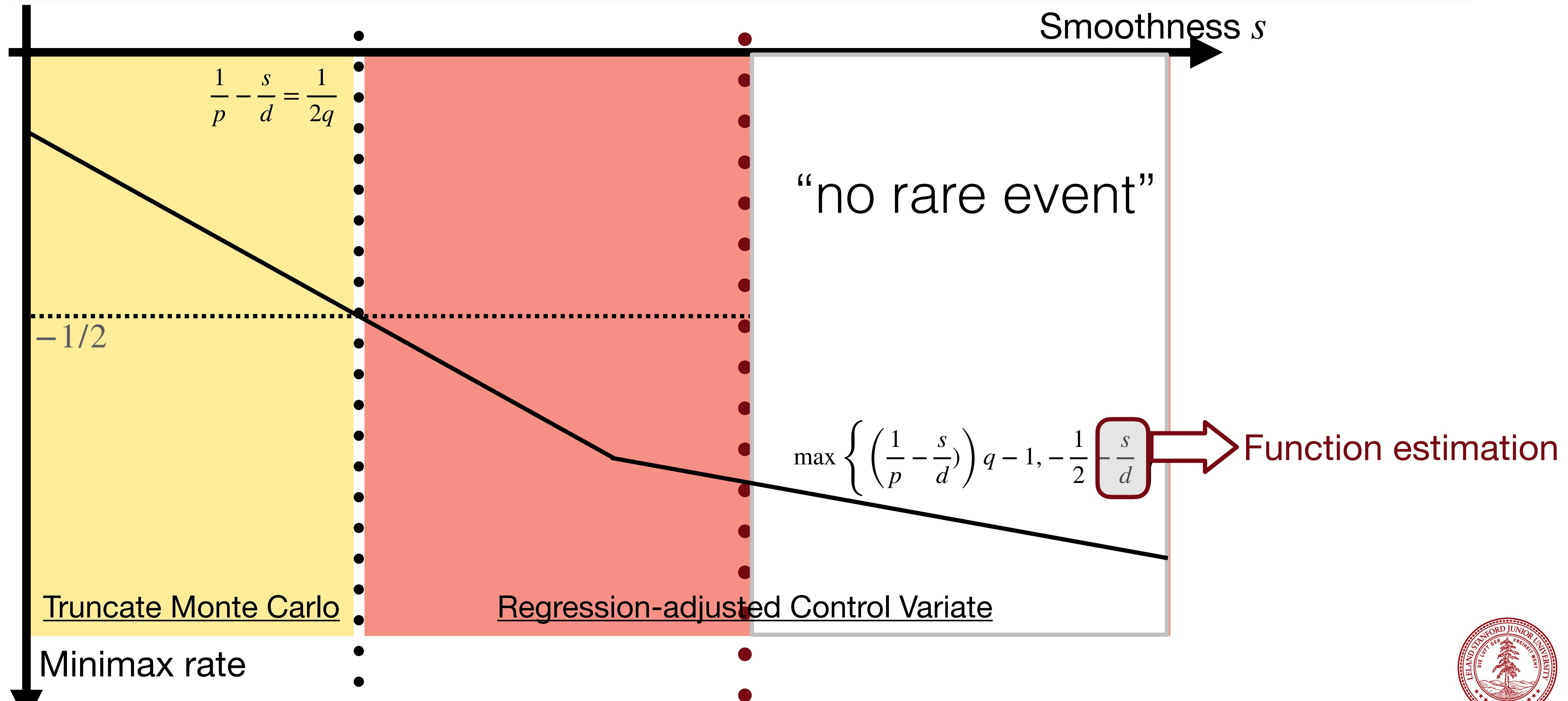
# When the control variate helps



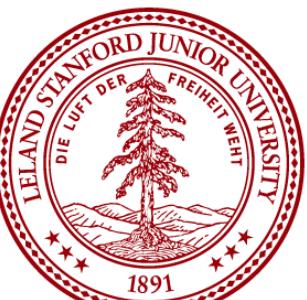
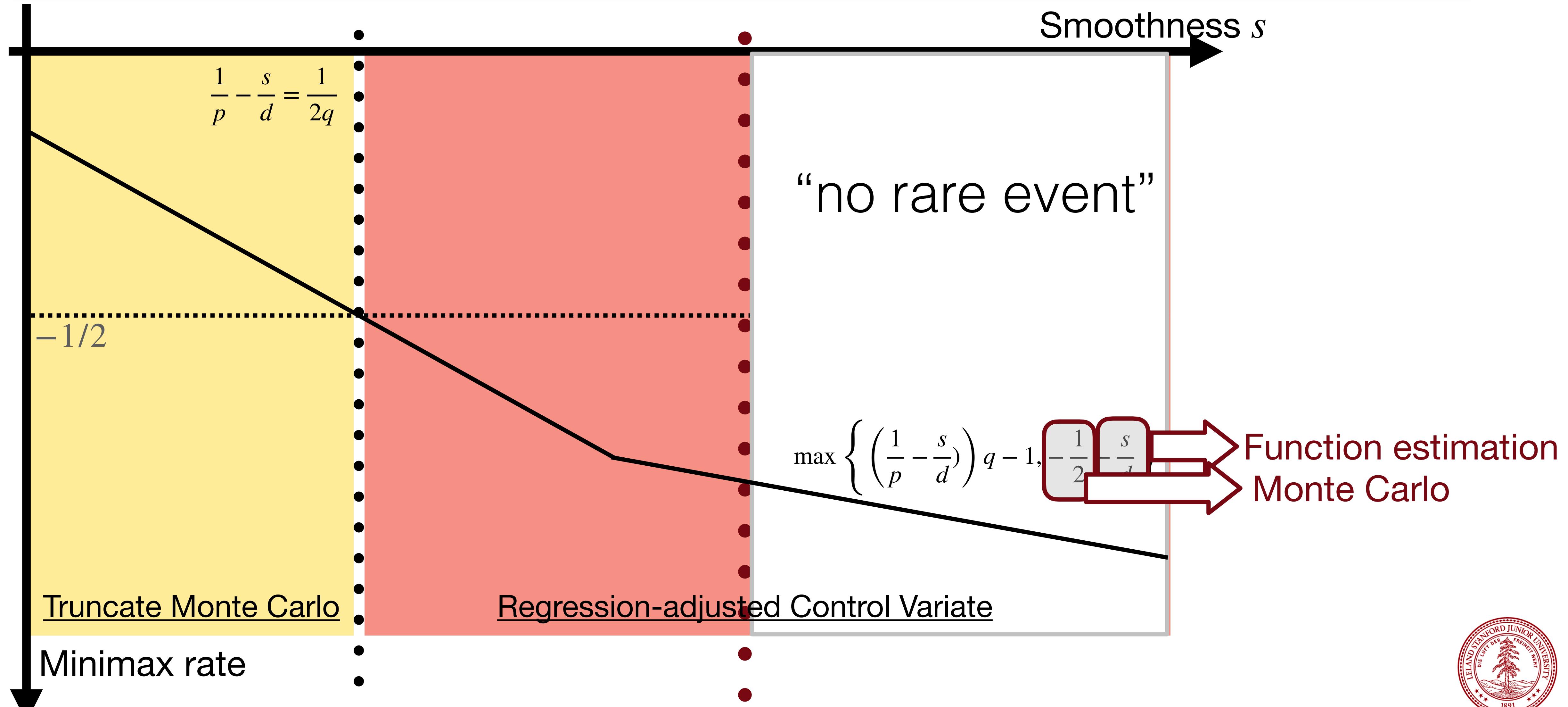
# When the control variate helps



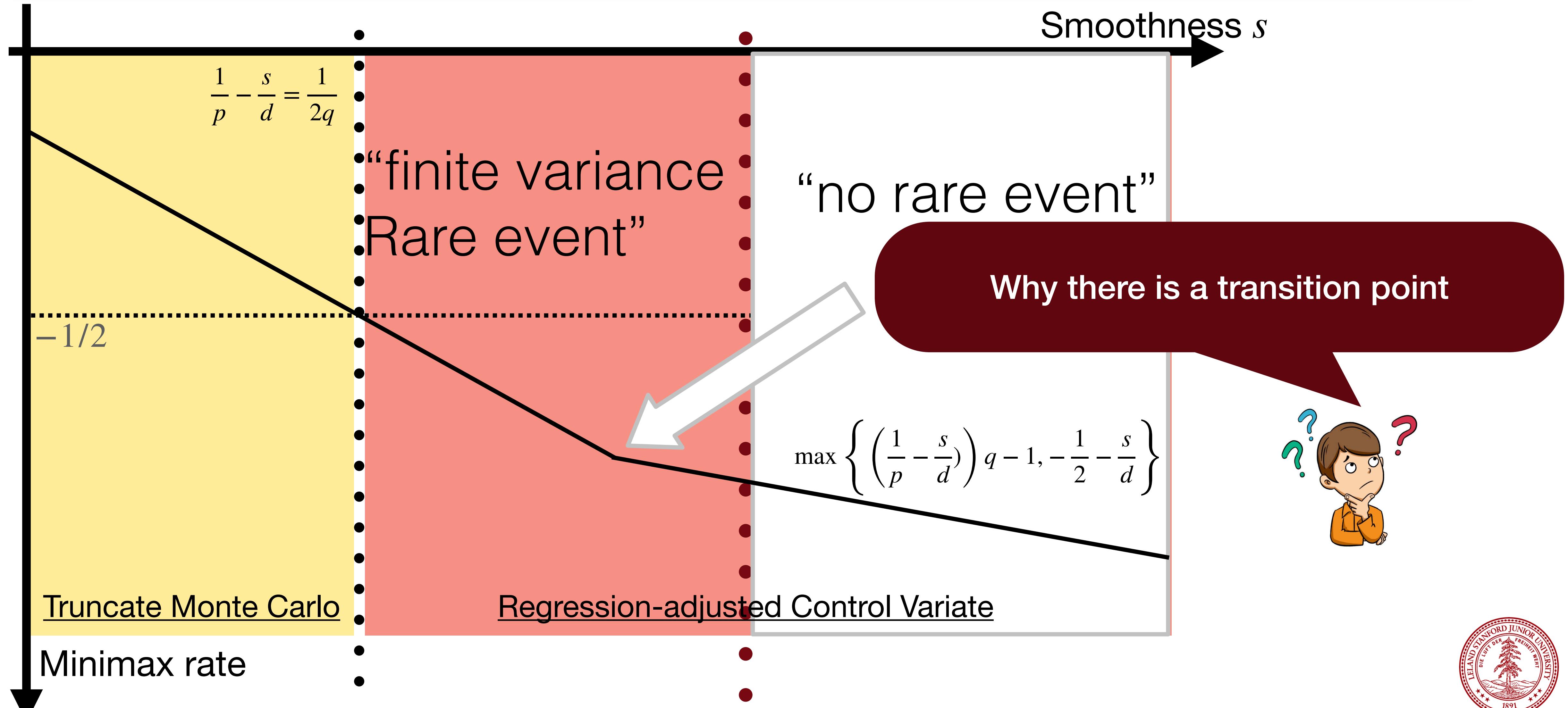
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# When the control variate helps



# When the control variate helps



# Semi-parametric efficiency...

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## Example

Monte Carlo Estimate  $\mathbb{E}_P f$      $\mathbb{E}_P f^q, f \in W^{s,p}$

## Step 1

Using half of the data to estimate  $\hat{f}$

## Step 2

$$\mathbb{E}_P f^q = \mathbb{E}_P (\hat{f})^q + \mathbb{E}_P (f - \hat{f})^q$$

**Low order term**

$$f^{q-1}(f - \hat{f}) + (f - \hat{f})^q$$

“influence function” (gradient)

# Semi-parametric efficiency...

## Example

Monte Carlo Estimate  $\mathbb{E}_P f \quad \mathbb{E}_P f^q, f \in W^{s,p}$

## Step 1

Using half of the data to estimate  $\hat{f}$

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$$\mathbb{E}_P f^q = \mathbb{E}_P (\hat{f})^q + \mathbb{E}_P (f - \hat{f})^q$$

**Low order term**

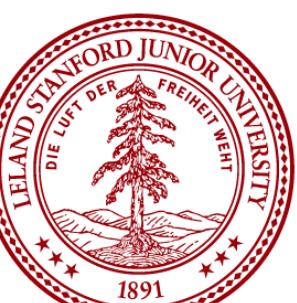
$$f^{q-1} (f - \hat{f}) + (f - \hat{f})^q$$

**“influence function” (gradient)**

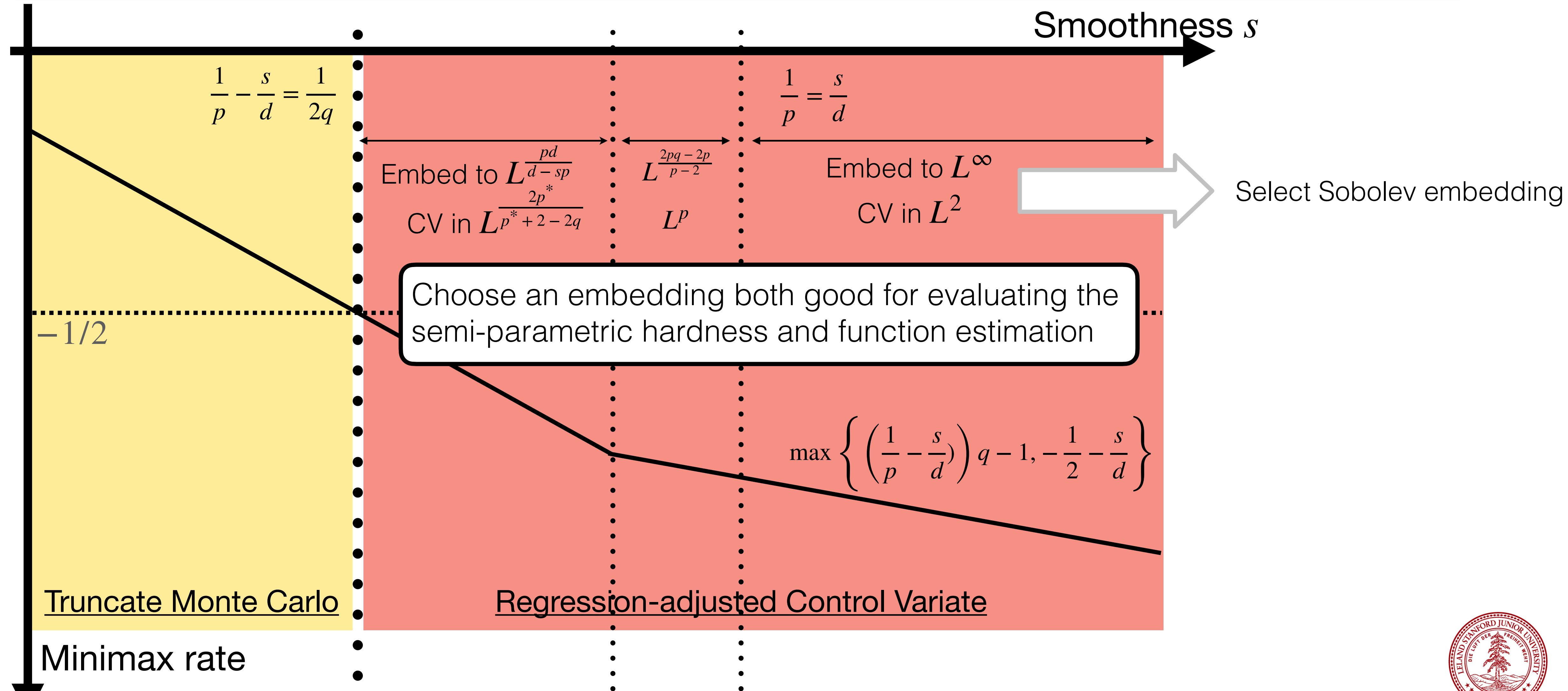
How to select the sobolev  
emebedding



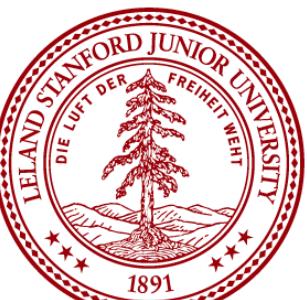
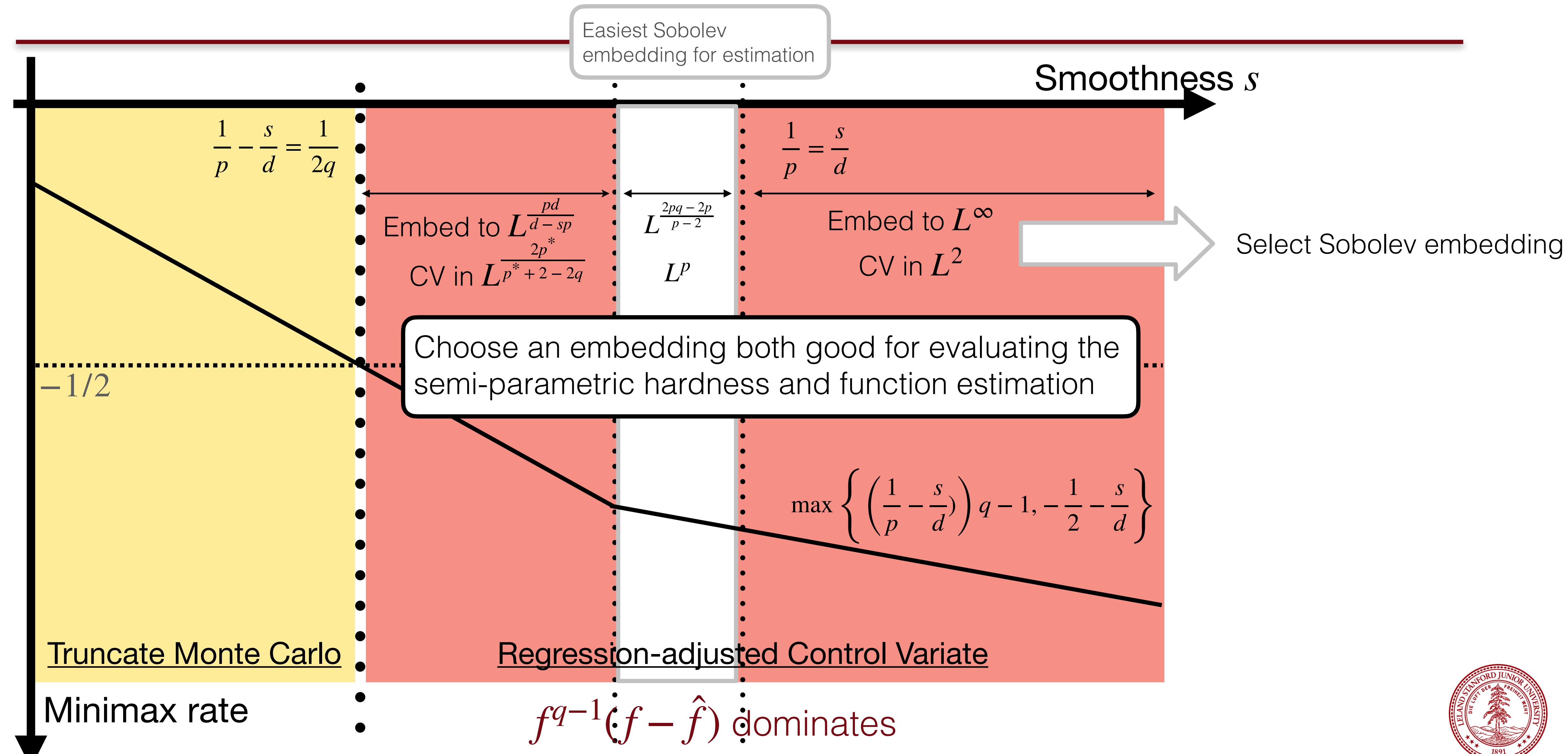
Embed  $f^{q-1}$  and  $f - \hat{f}$  into “dual” space



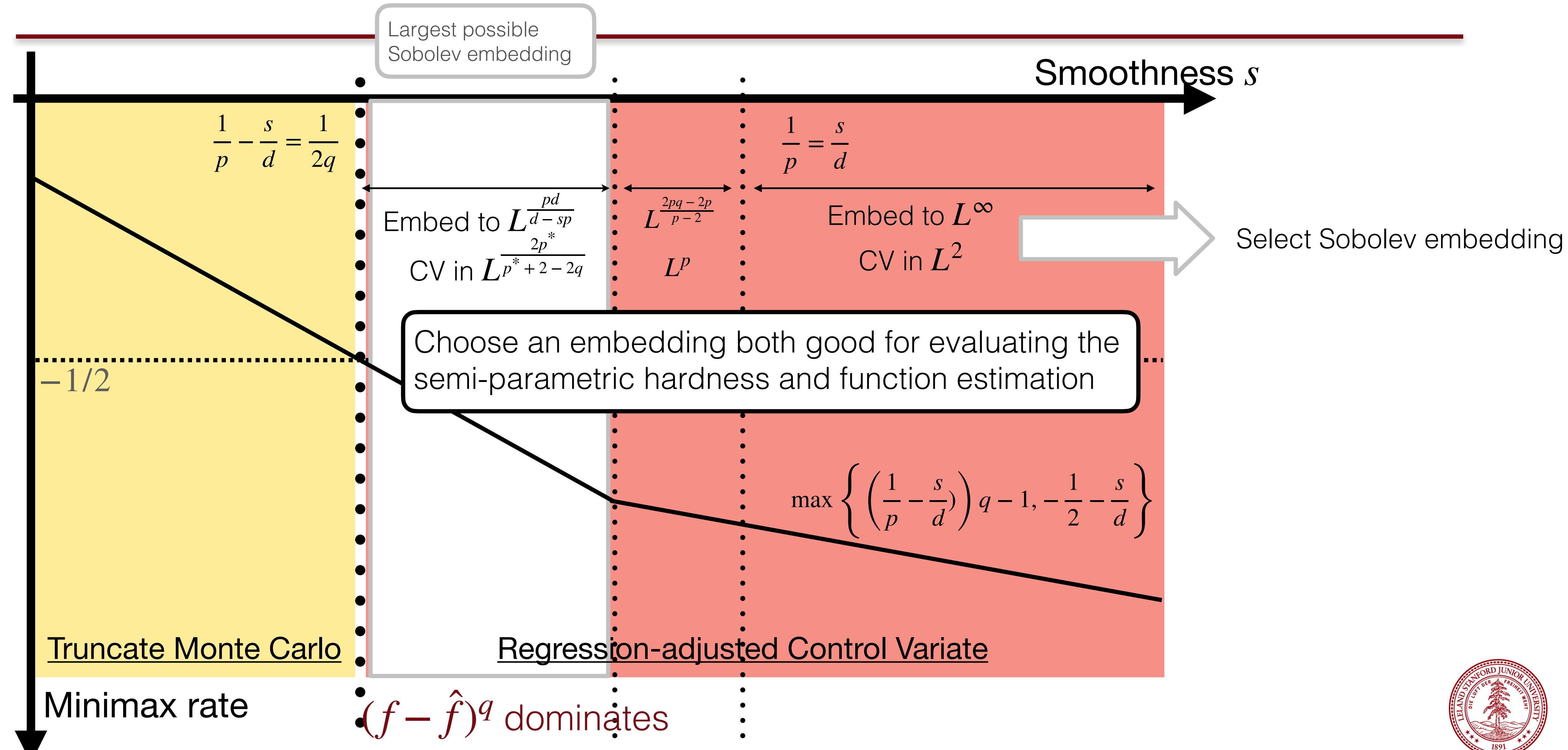
# Tricky part of the Proof:select embedding



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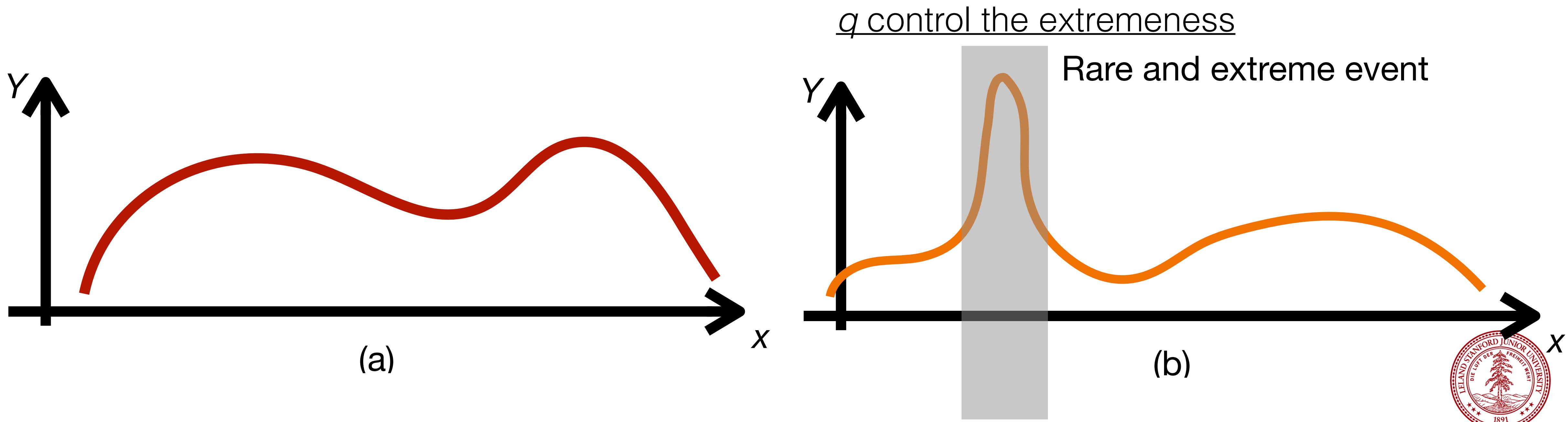
# Tricky part of the Proof:select embedding



# Take home message

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- a) Statistical optimal regression is the optimal control variate
- b) It helps only if there isn't a hard to simulate (infinite variance)  
Rare and extreme event





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