Module 10: Response Surface Methodology

DAV-6300-1: Experimental Optimization

David Sweet // 20241114

Review: Thompson sampling

- Allocate observations to arms in proportion to the probability each arm is best
  - $p_{\text{arm}} \propto p_{\text{best}}$
- Stop when $\max\{p_{\text{best}}\} > 0.95$

Review: A/B Test

- Goal: Accept or reject B
- Design: $N \geq (\frac{2.5\hat{\sigma}_\delta}{PS})^2$
- Measure: Replicate (reduce variance), Randomize (reduce bias)
- Analyze:

Criterion 1: $\delta > 1.6se \;\; (t > 1.6)$

Criterion 2: $\delta > PS$

Review: Law of Large Numbers

- N observations, y_i, the business metric
- w/mean $\mu = \frac{\Sigma_i^N y_i}{N}$
- As $N \rightarrow \infty$, $\mu \rightarrow E[y]$
- IOW: Our measurement (μ) estimates the true, unobservable business metric

Key Terms

- Surrogate
- Response surface
- OFAT (One Factor At a Time)

Case: Song recommender

- In prod (A): Ranking songs by p_{listen} = P{user will listen until the end}
- In dev (B): Ranking songs by p_{like} = P{user will click song's like button}
- A/B test the two models?
- Why not use both? Rank by a score:

$$score = wp_{\text{listen}} + (1 - w)p_{\text{like}}$$

Case: Song recommender

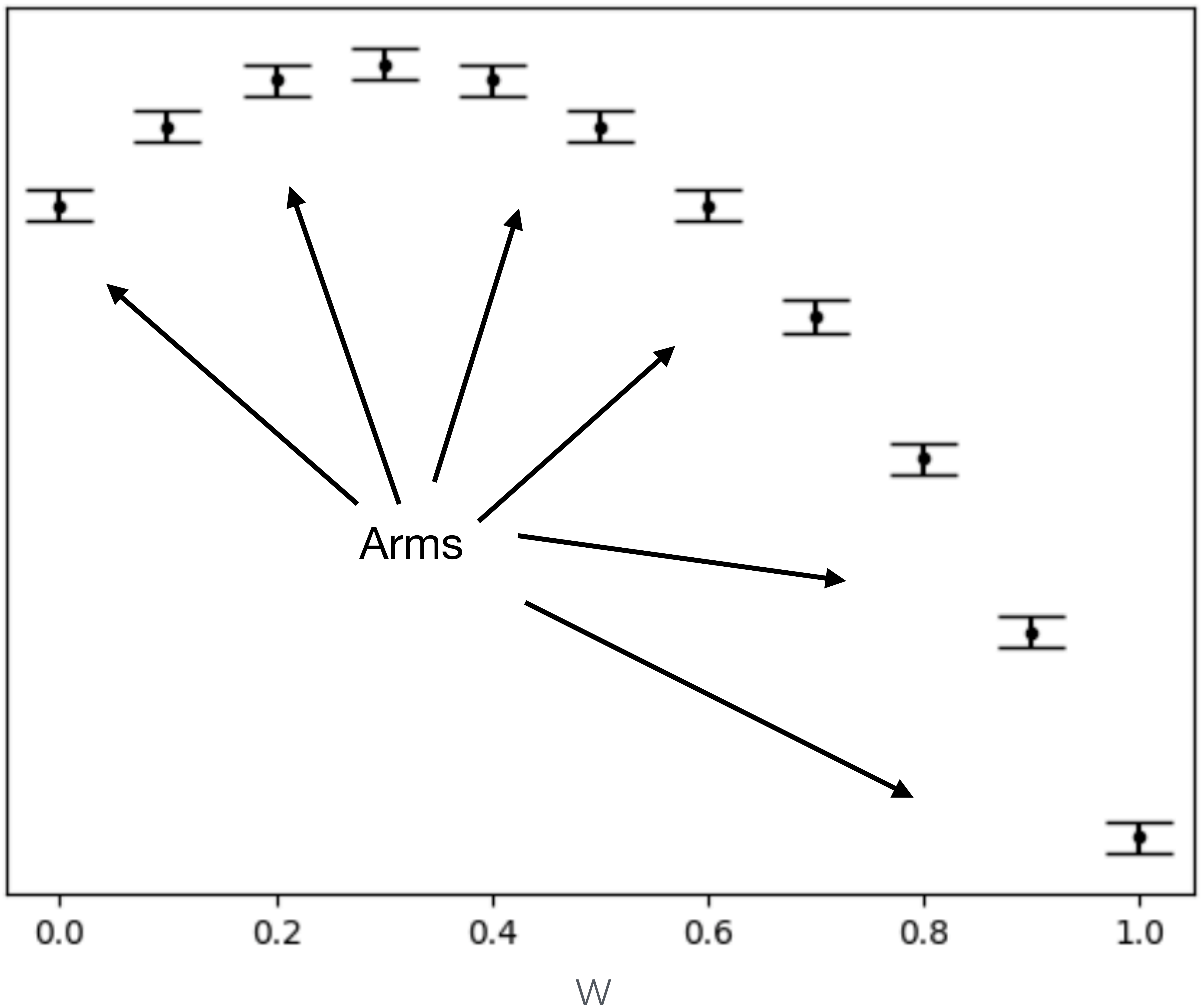
- Combine models, $w \in [0,1]$

$$score = wp_{\text{listen}} + (1 - w)p_{\text{like}}$$

- Find w that gives highest BM
  - … via experimental optimization

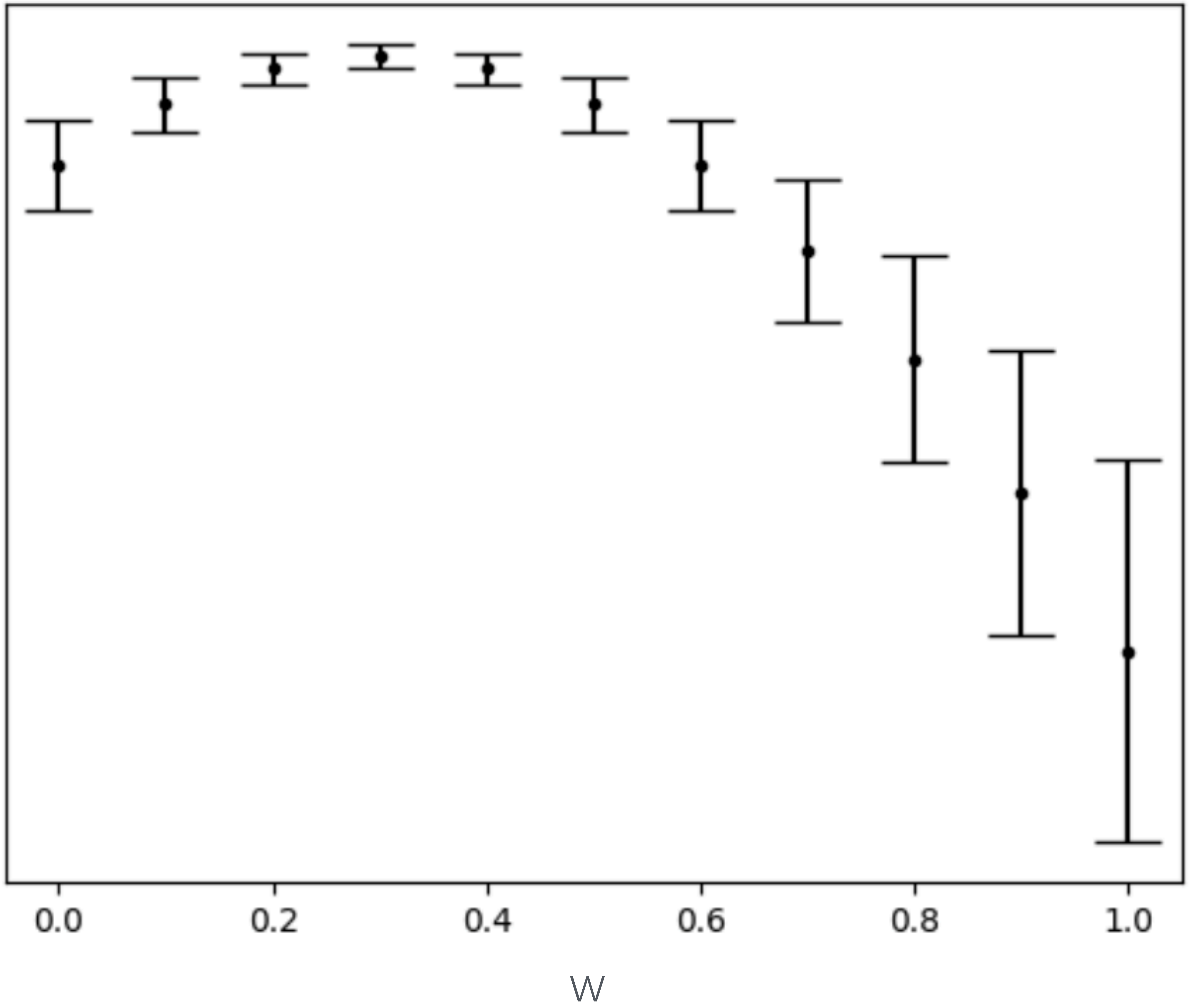
Case: Song recommender

- Approach I: A/B/n test
- Measure $w \in \{0, 0.1, 0.2, \ldots, 1.0\}$
- Req. many observations:
  - Lots of capacity
  - Bonferroni



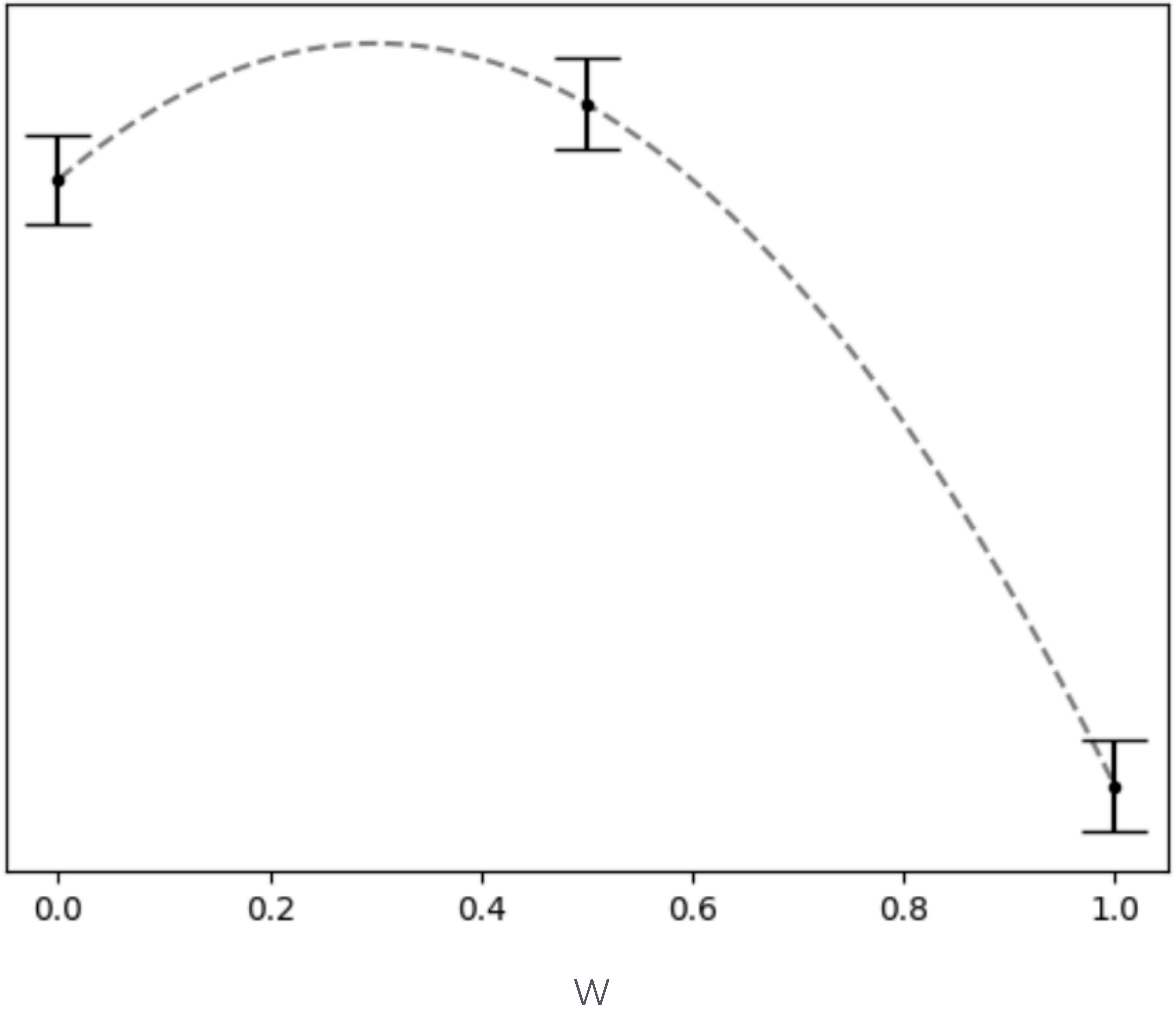
Case: Song recommender

- Approach II: Multi-armed bandit
- Same number of arms
- Fewer observations than A/B/n:
  - Worse arms are allocated fewer observations



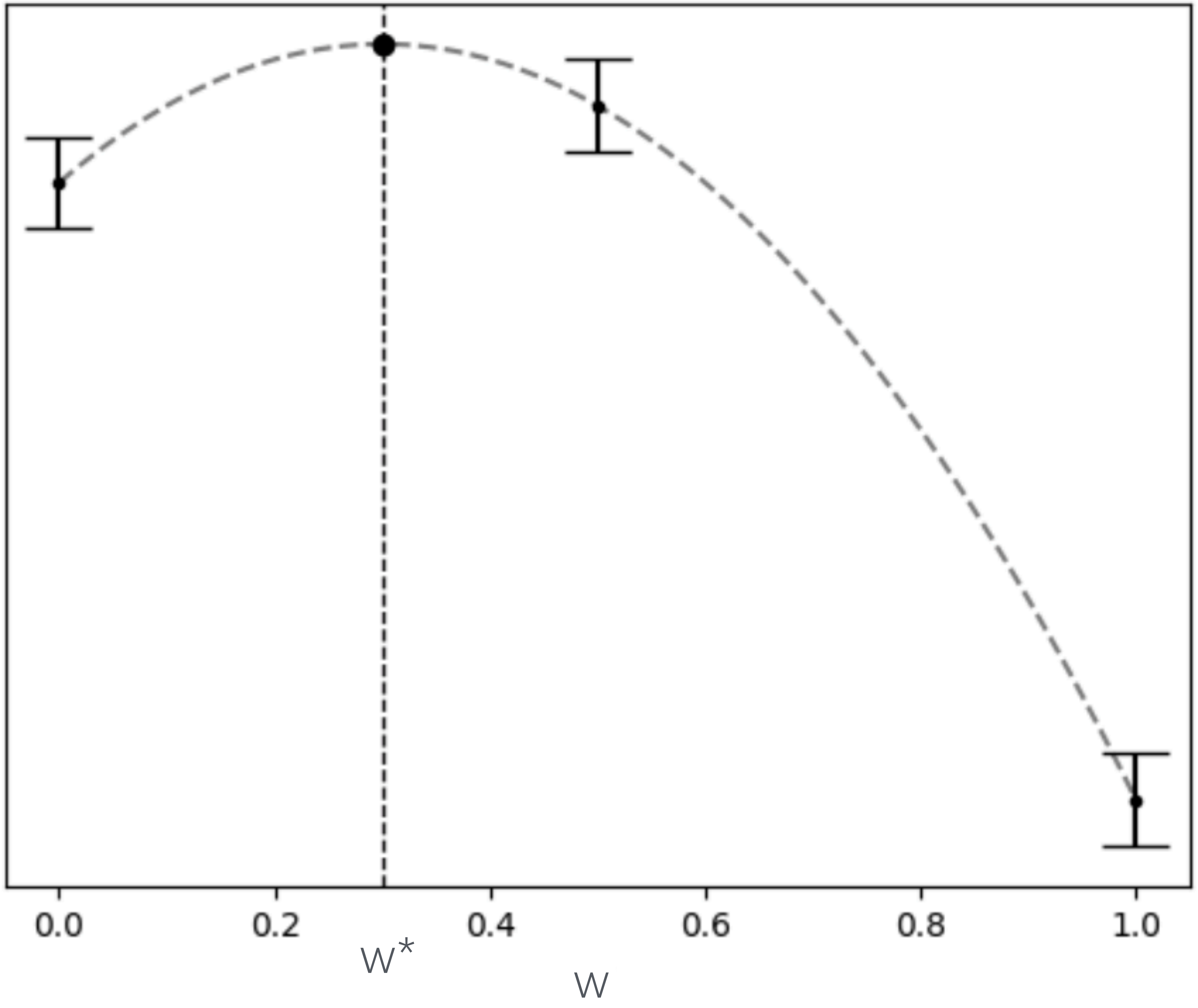
Case: Song recommender

- Measure only three arms: $w \in \{0, 0.5, 1.0\}$
- Fit a parabola
- Guess/hope that max of parabola is true (expected) max



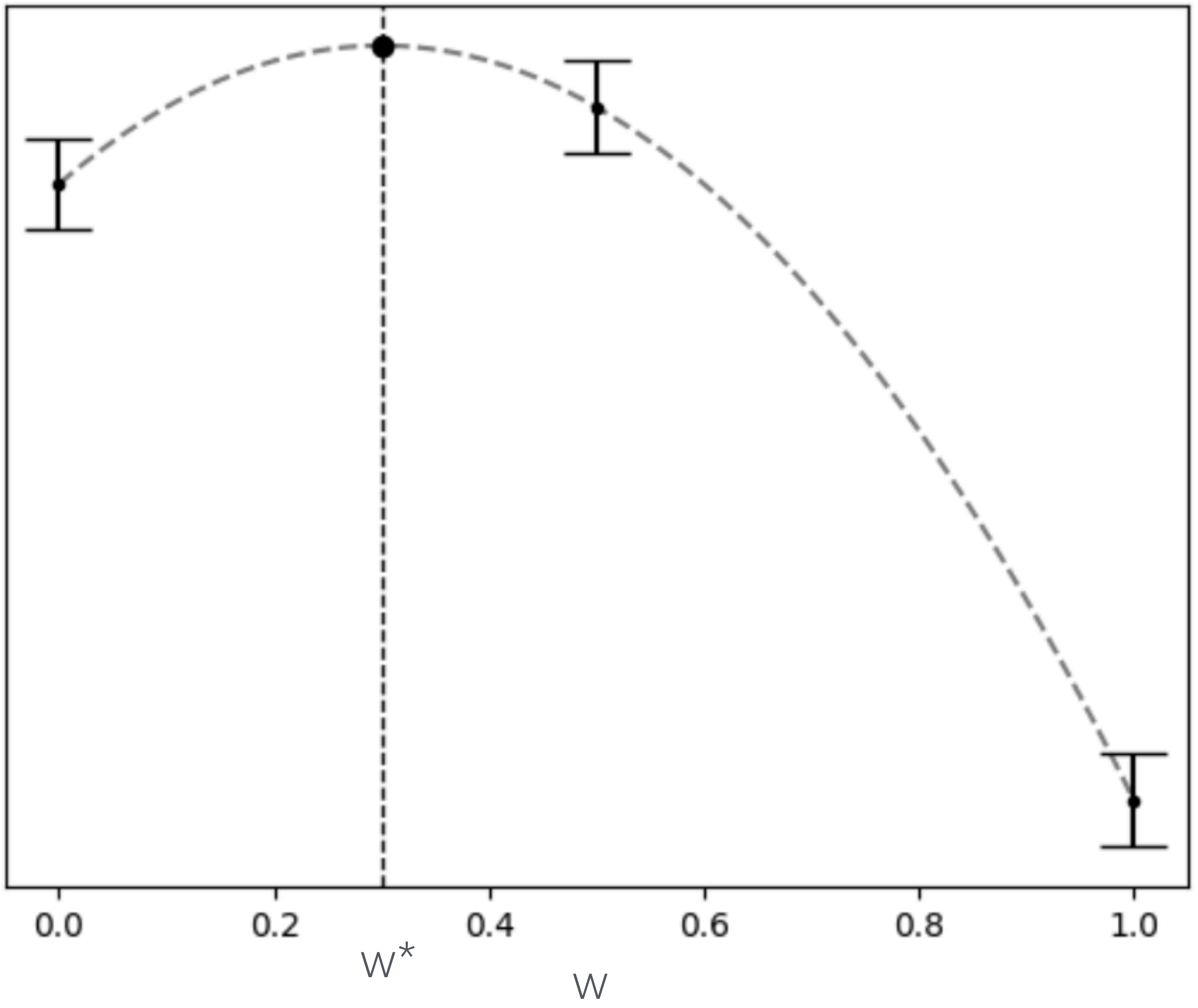
Case: Song recommender

- Max of parabola: $w = 0.3$
- Run A/B test:
  A: Current prod version
  B: $w = 0.3$
- A/B test validates inference
  (or *in*validates)



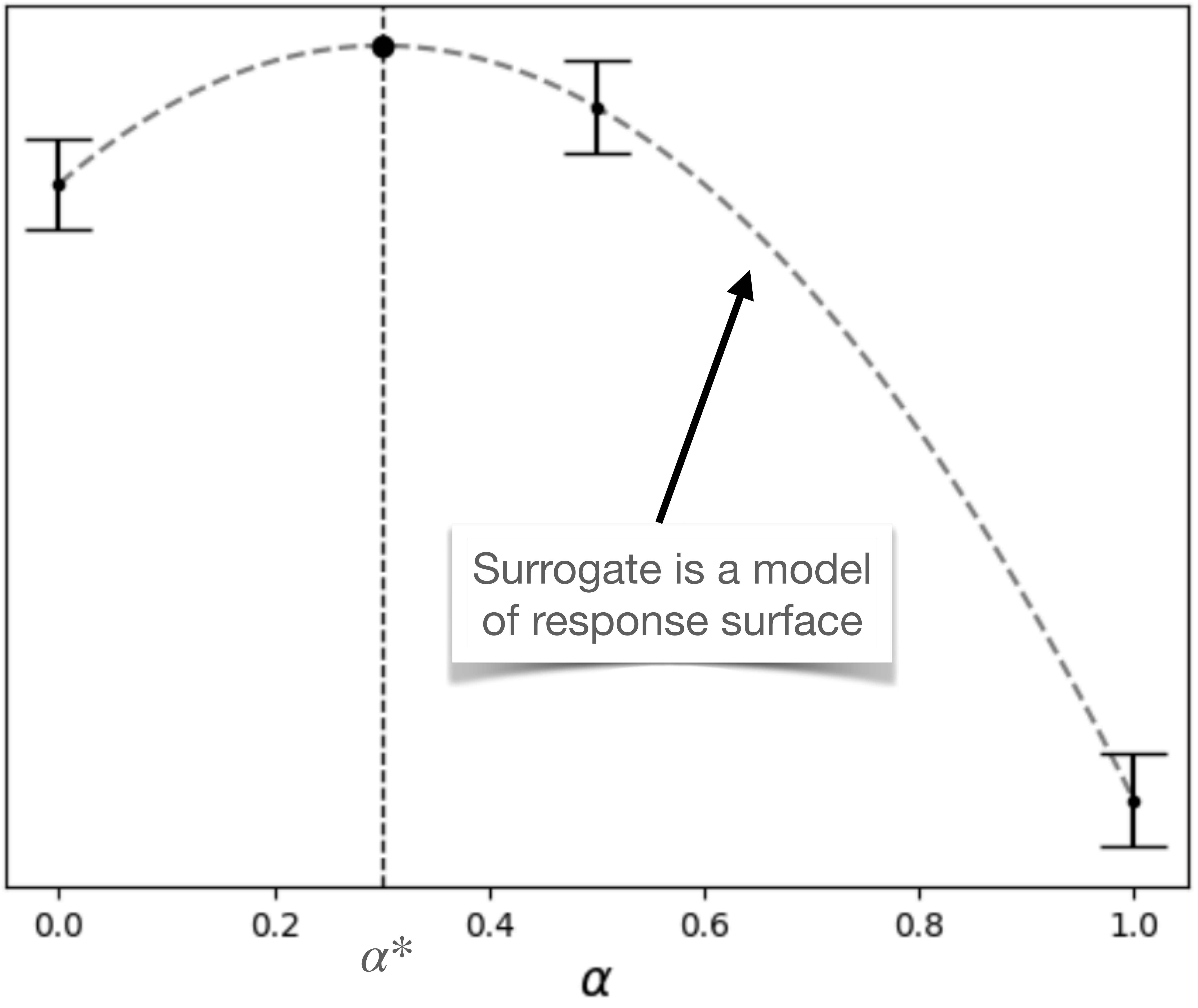
Case: Song recommender

- True function being modeled is $E[BM]$ vs. w
- Model estimates function
  - y axis: estimated BM, $y(x)$
  - x axis: parameter, w



Case: Song recommender

- Unobservable, "true" BM function, $E[BM]$, called *response surface*
- Our fit parabola, $y(x)$, called *surrogate function*
- *Response surface method:*
  - Model, optimize, validate



Compare A/B test to RSM

- A/B tests and MABs compare distinct versions of system
- RSM compares continuous family of systems
  - IOW, RSM finds optimal value of a continuous parameter

A/B Test	**RSM**
BM	BM
BM(A), BM(B)	BM(x)
$y, E[y]$	$y(x), E[y(x)]$

Compare A/B testing to RSM

- Parameter types:
  - Categorical: A, B, C, ...; true/false; red/green/blue; low/medium/high
  - Ordinal: 1, 2, 3, 4, ...
  - Continuous: [0.0, 1.0]; [-3.14, 3.14]; real, double, float
- Think of
  - A/B testing as optimization over a categorical parameter
  - RSM as optimization over a continuous parameter

Validate optimum

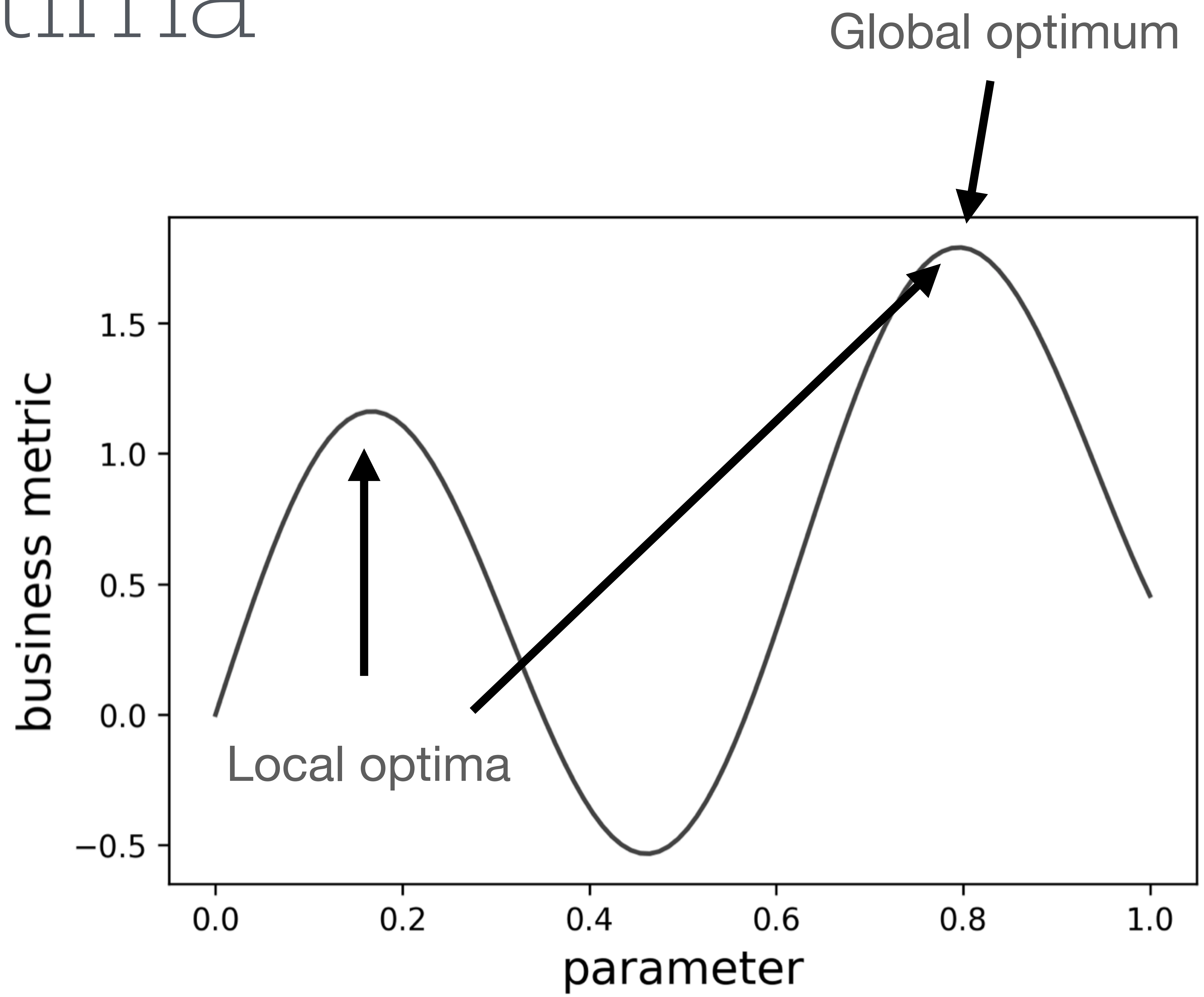
- Surrogate (model of RS) is only an approximation
- Validate by measuring at the predicted-best parameter
    - A/B test (or MAB) just best vs. old prod

Use N from A/B testing

- RSM measurements are aggregate measurements
- Use $N = (\frac{2.5\hat{\sigma}}{PS})^2$
- PS here says “If the BM of two parameters is within PS, I’ll treat them as equivalent”
- Alternatively, “I want to be within PS of the true optimum”

Local vs. global optima

- Response surface might have multiple humps
- You want the highest hump
- RSM will only search locally
- Think hard about parameter range
- Local optimum is better than nothing

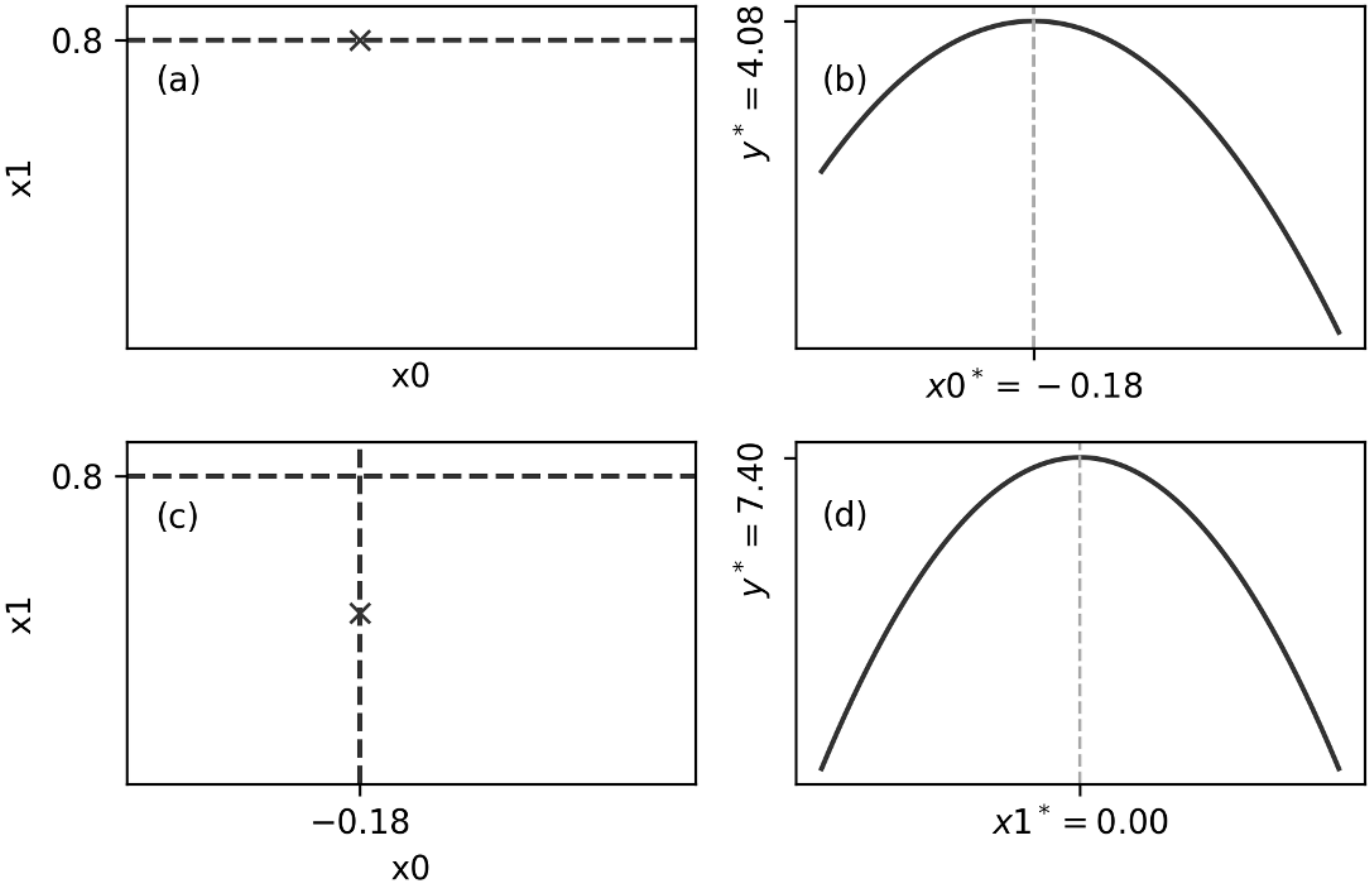


Interactive, manual process

- Engineer chooses
  - *Region of interest* (ROI): range of parameter(s) to investigate
  - Design of experiment: which specific parameter values to measure
  - Form of model — parabola? multiple parameters
- May make decisions via visualization of surrogate
- ROI “recentered” on each iteration

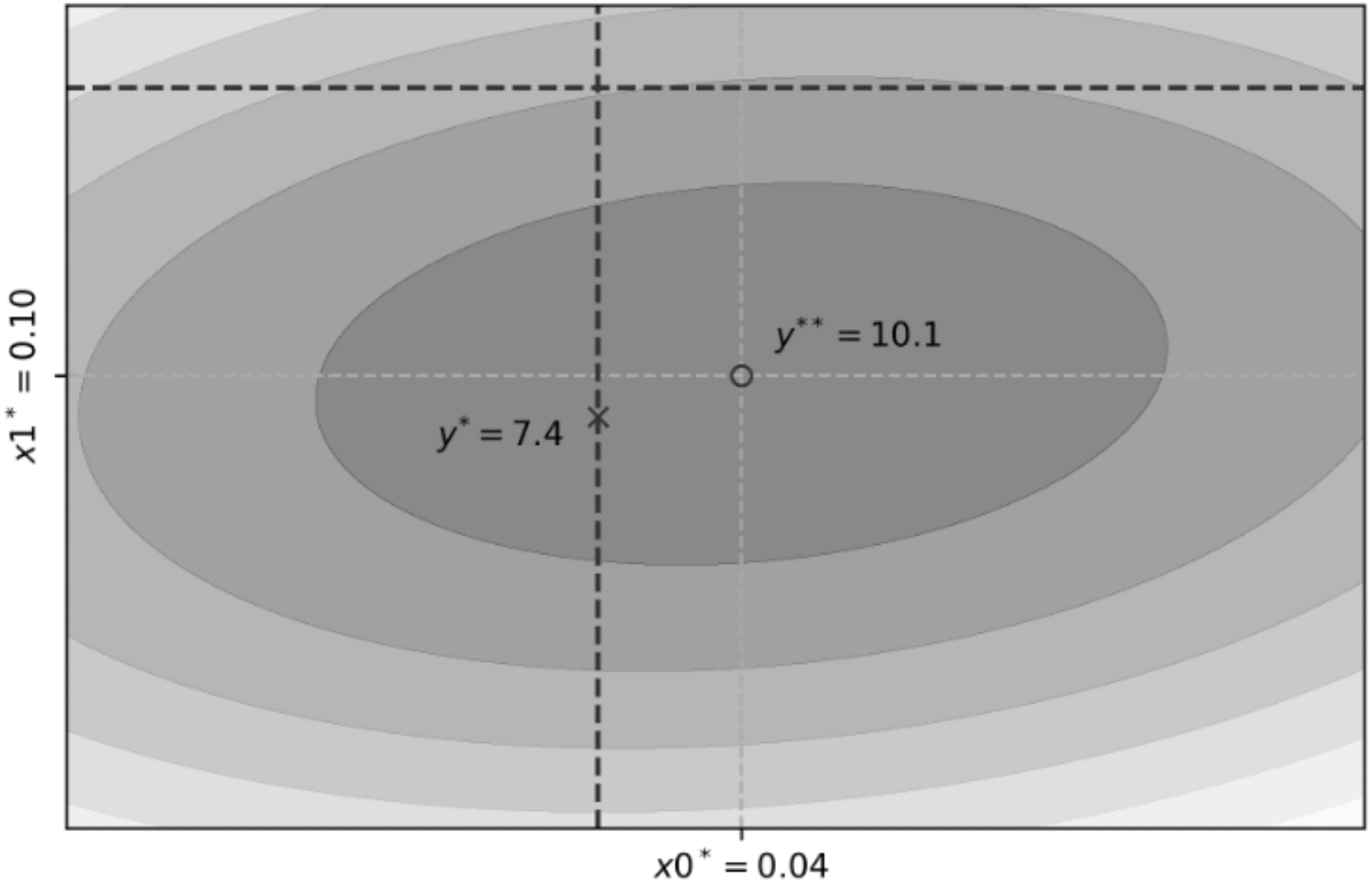
Multiple parameters

- Ex x_0, x_1
- Optimize x_0
- Optimize x_1
- *OFAT: One factor at a time*
    - Suboptimal approach



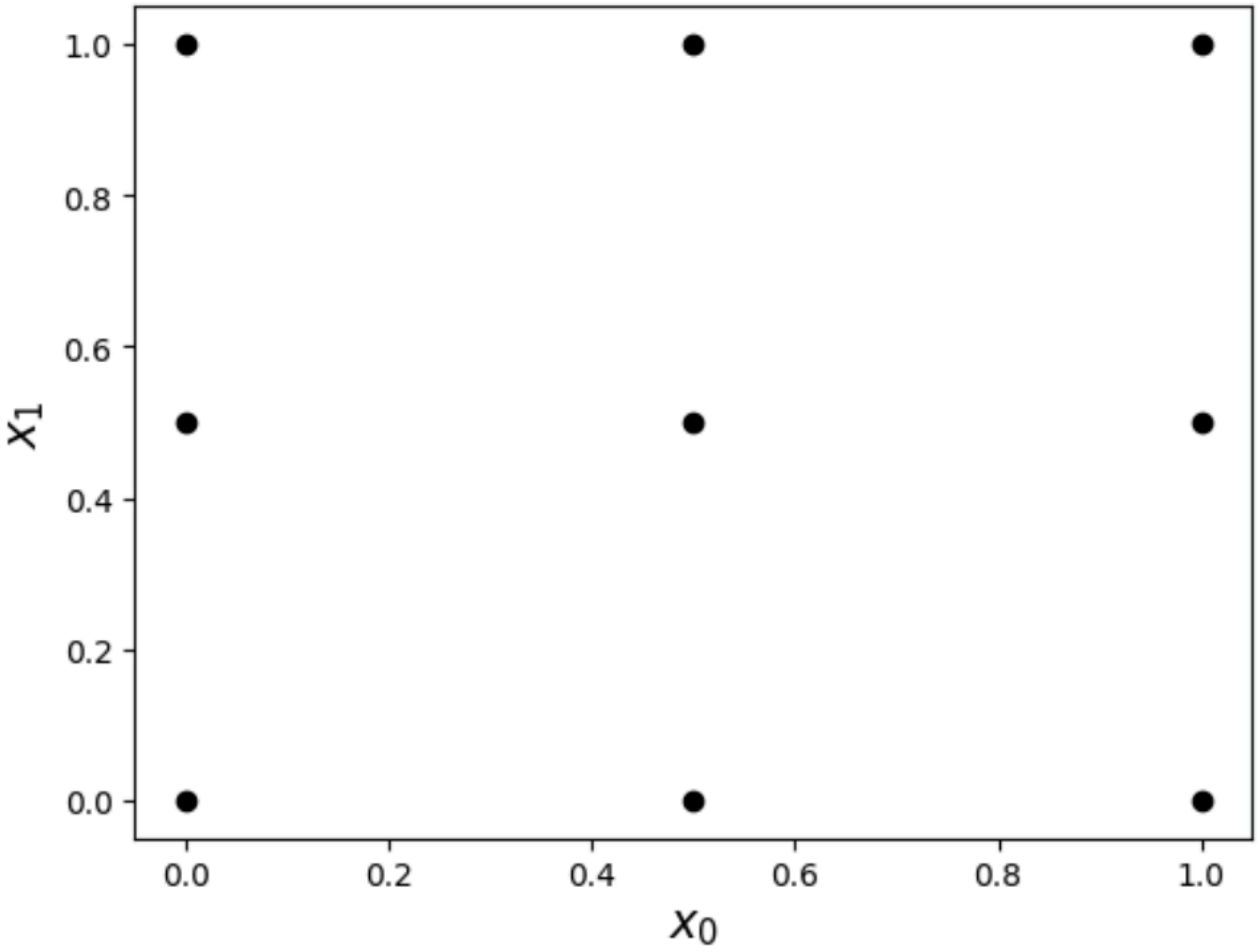
Multiple parameters

- OFAT finds $y^* = 7.4$
- RSM applied simultaneously to x_0, x_1 finds $y^* = 10.1$
- Realistically:
  - System has **many** parameters
  - "A few at a time" is typically as good as it gets



Two-parameter RSM

- Two parameters (*dimensions*)
  - Take 9 measurements on a grid
  - Fit surrogate $y(x_0, x_1)$
  - Optimize to find x_0^*, x_1^*
  - A/B test
    A=current, B=x_0^*, x_1^*



Linear regression surrogate

- Surrogate model: linear regression
- Ex: $y = \beta_0 + \beta_1 x + \varepsilon$

Measurements, not observations

  - Take measurements $\{(y_0, x_0), (y_1, x_1), (y_2, x_2), \ldots (y_m, x_m)\}$
  - Fit model

$$\beta_0 = \frac{\sum_i y_i}{m}, \beta_1 = \frac{\sum_i x_i y_i}{\sum_i x_i x_i}$$

- Parabola: $y = \beta_0 + \beta_1 x + \beta_2 x^2 + \varepsilon$

Linear regression surrogate

- Two parameters (dimensions, 2D)
- $y = \beta_0 + \beta_{1,0}x_0 + \beta_{1,1}x_1 + \beta_{2,0,0}x_0^2 + \beta_{2,1,1}x_1^2 + \beta_{2,0,1}x_0x_1 + \varepsilon$
- notation: $y \sim x_0 + x_1 + x_0^2 + x_1^2 + x_0x_1$
- even better: $y \sim \sum_i^2 x_i + \sum_i^2 \sum_j^2 x_ix_j$

Linear regression surrogate

$$y \sim \sum_{i}^{2} x_i + \sum_{i}^{2} \sum_{j}^{2} x_i x_j$$

- Fit: $\vec{\beta} = (X^\top X)^{-1}(X^\top y)$

First column of X is all ones

- NumPy: `beta = np.linalg.inv(X.T @ X) @ (X.T @ y)`
- Works for any number of dimensions (parameters)

Linear regression surrogate

- More parameters
  - 3D: $y \sim \sum_{i}^{3} x_i + \sum_{i}^{3} \sum_{j}^{3} x_i x_j$
  - d dimensions: $y \sim \sum_{i}^{d} x_i + \sum_{i}^{d} \sum_{j}^{d} x_i x_j$
- Too many terms for only a few measurements
- Use automated variable selection and/or domain knowledge to limit terms

Summary

- RSM introduces
  - Surrogate: model of response function
  - Optimization of surrogate
- RSM is interactive/manual
  - Engineer decides ROI, design, and form of surrogate
- A/B testing : categorical :: RSM : continuous