Revisiting minimum description length complexity for overparameterized models

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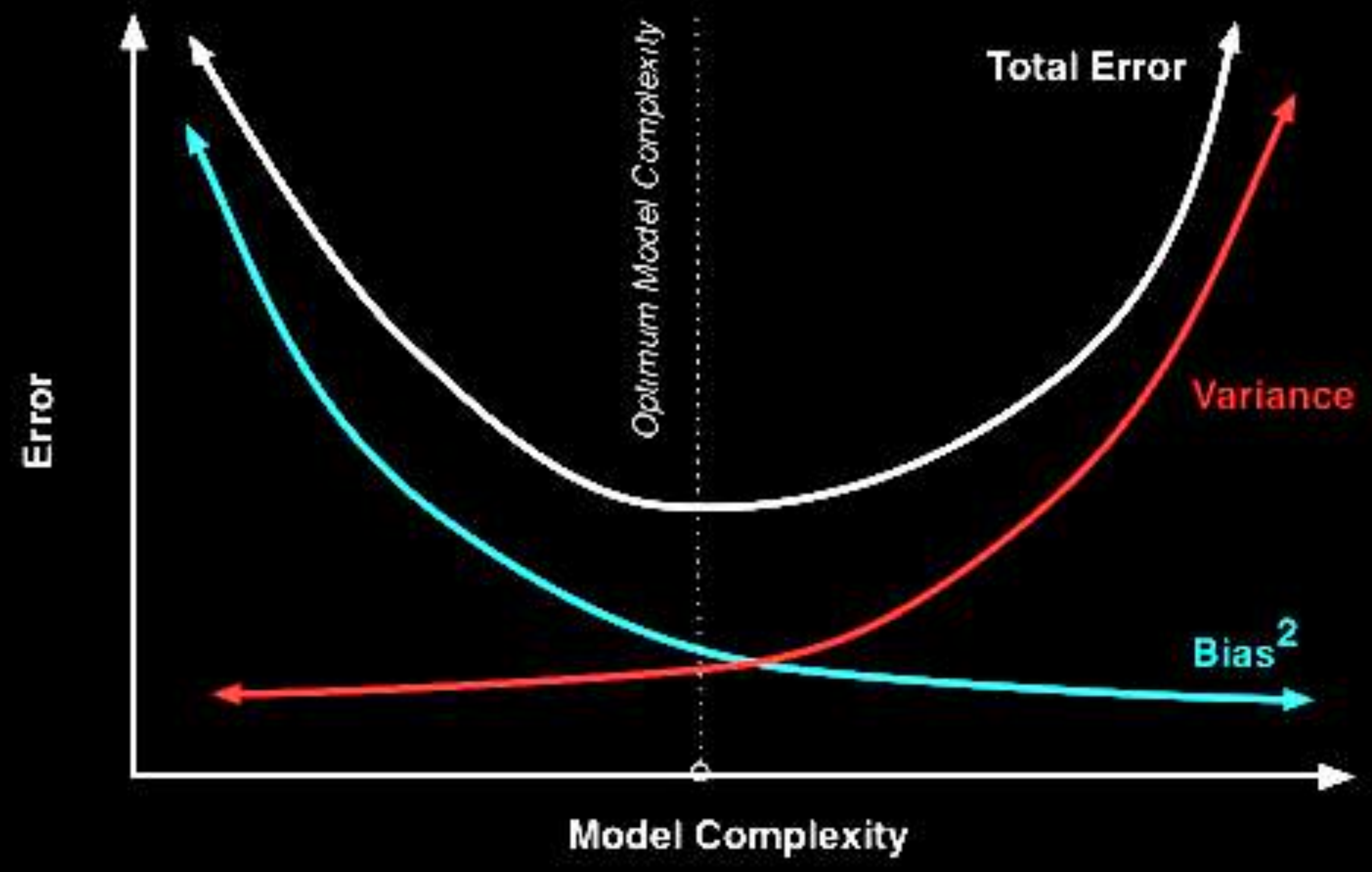
Classical Wisdom: **Occam's razor**

Use the simplest model that fits the data

U-shaped bias-variance tradeoff:

Low-dimensional settings with "good" estimators



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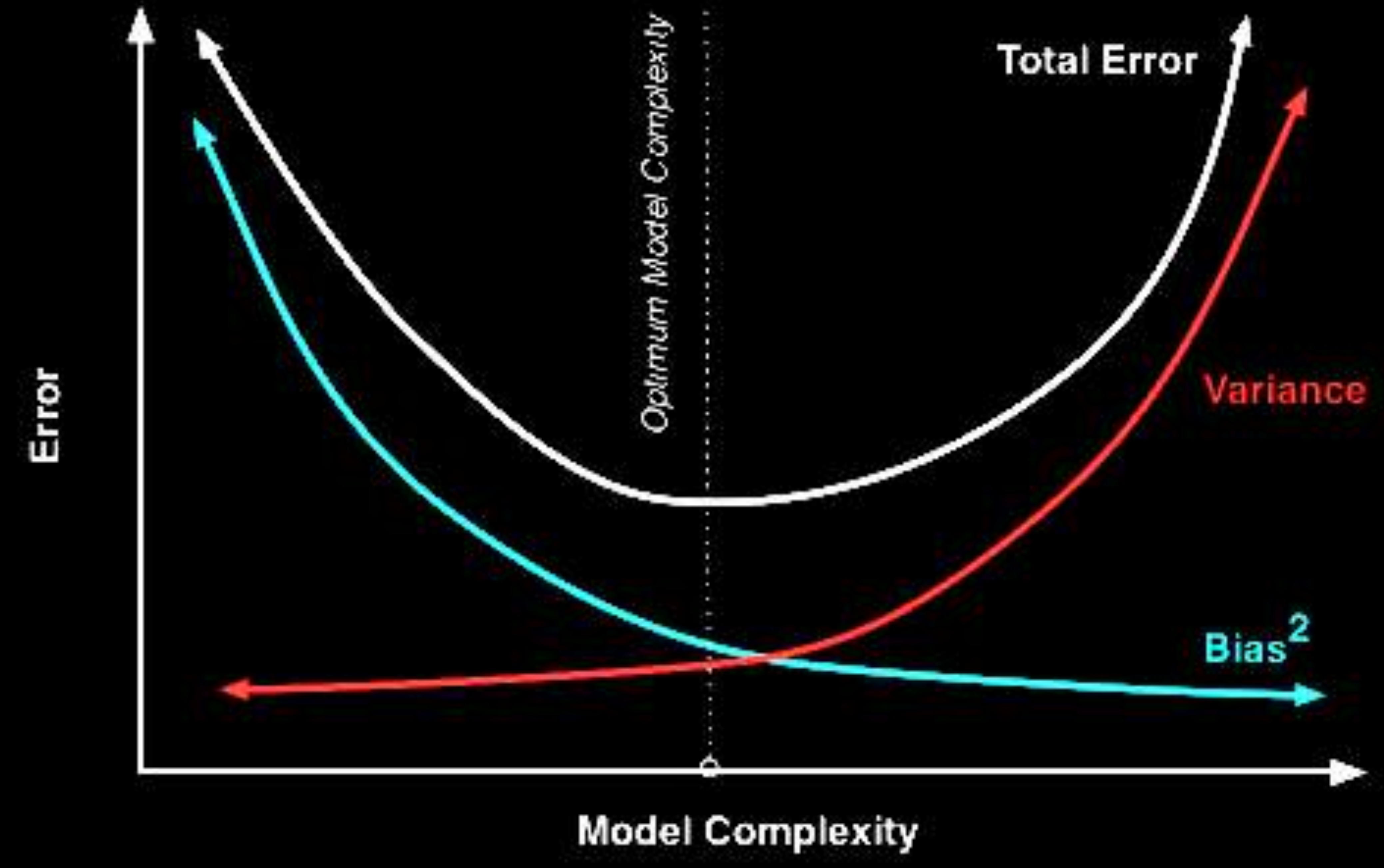
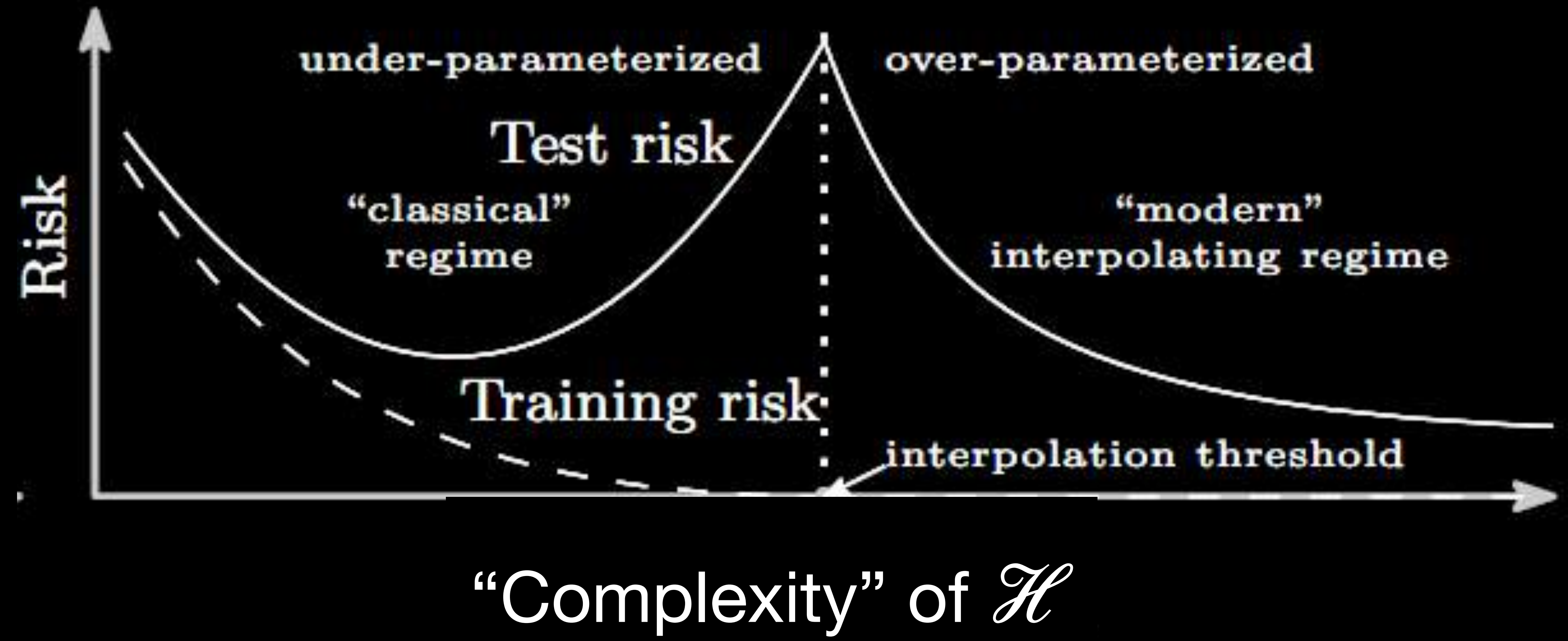


Modern Phenomenon: **Fit without fear!**
Use the largest model that achieves zero training error

Non-U shaped risk curves in modern overparameterized models



…, Skurichina-Duin 98,00, Belkin-Hsu-Ma-Mandal 18, Muthukumar-Vodrahalli-Sahai 19, Hastie-Montanari-Rosset-Tibshirani 19, …

Is double descent a conundrum for the classical wisdom?

We expect the classical U-shaped tradeoff given a **fixed dataset**, and as the "**complexity**" of the fitted estimator varies

d = number of features

n = number of samples

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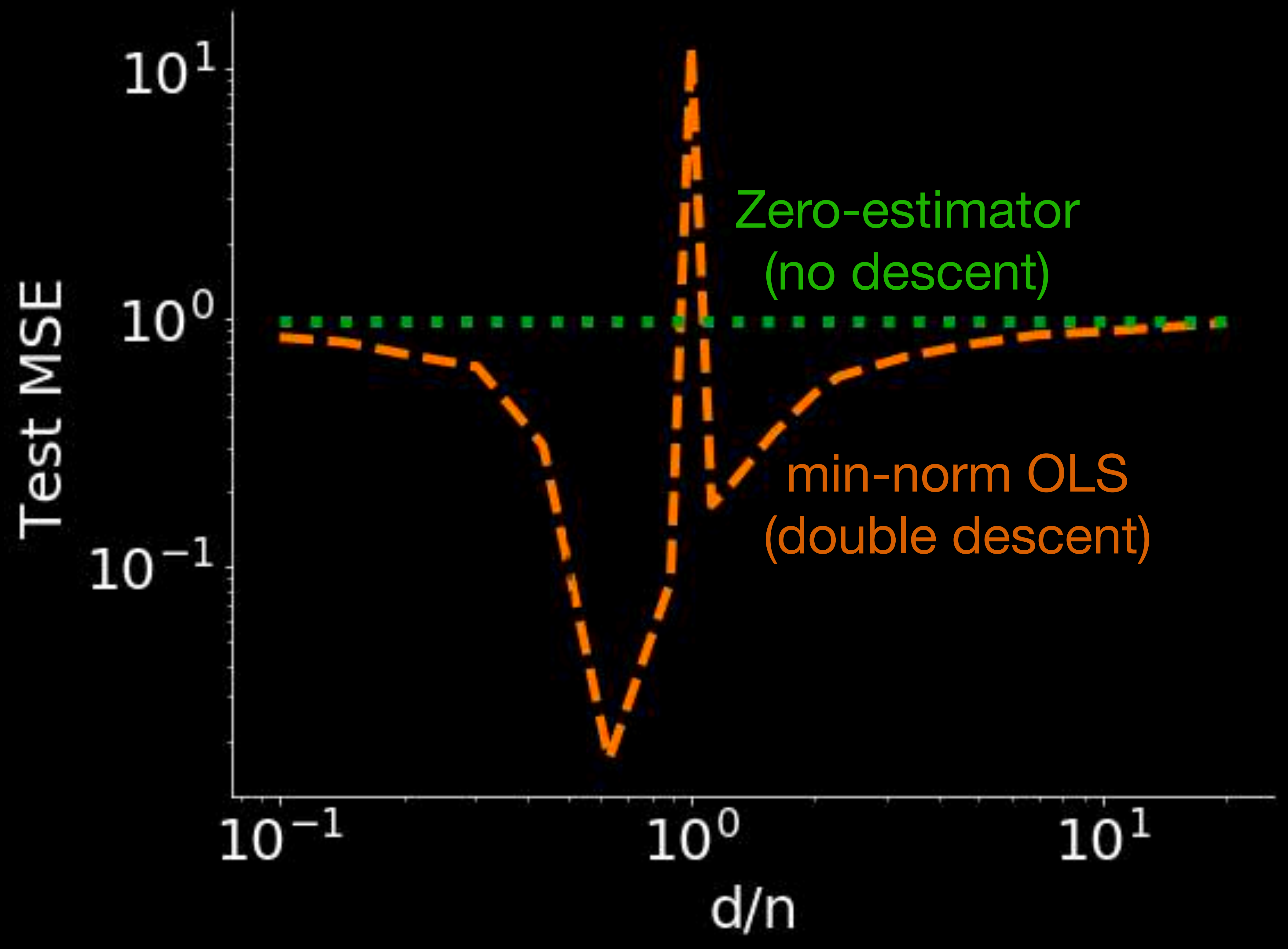

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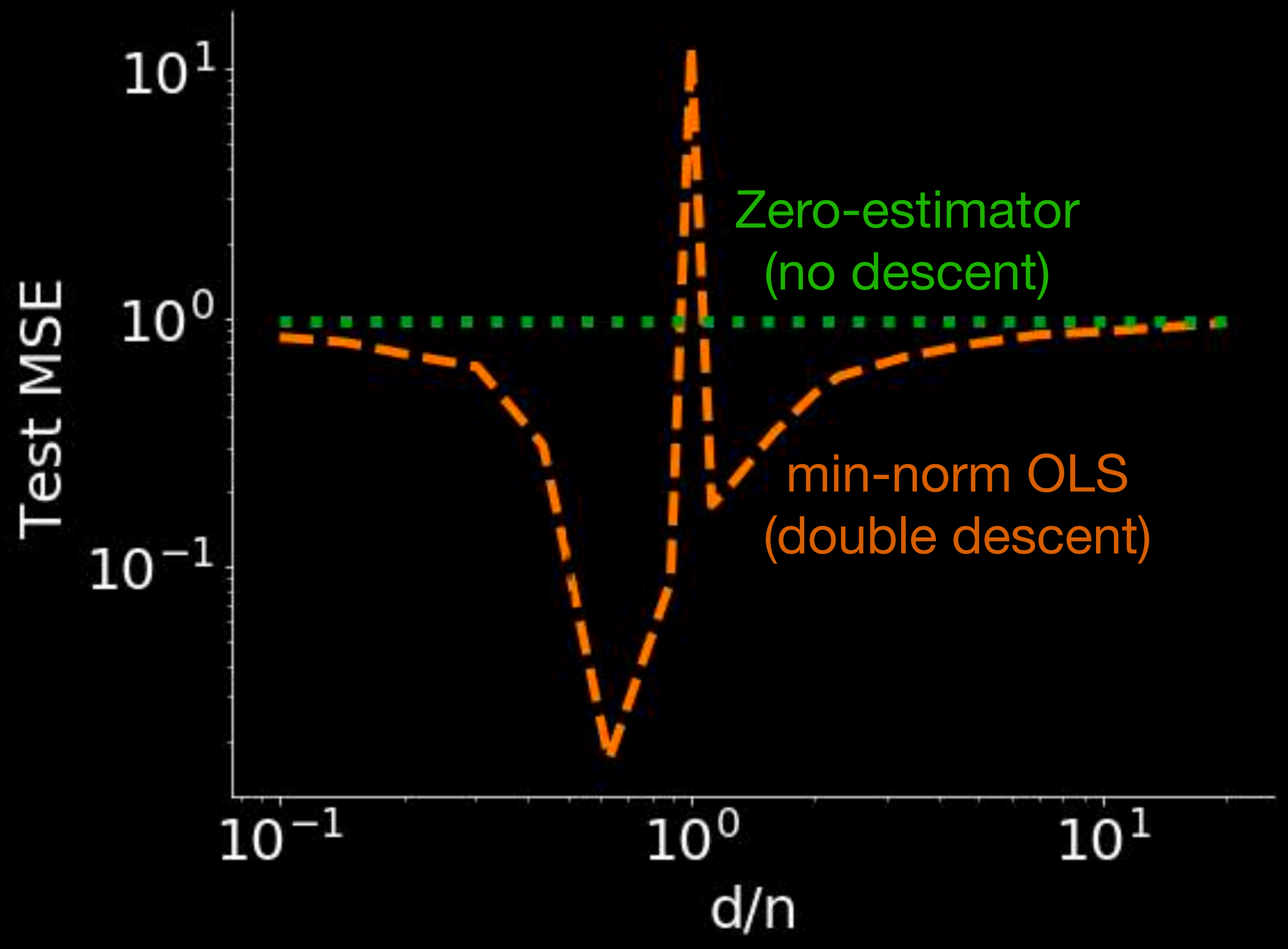

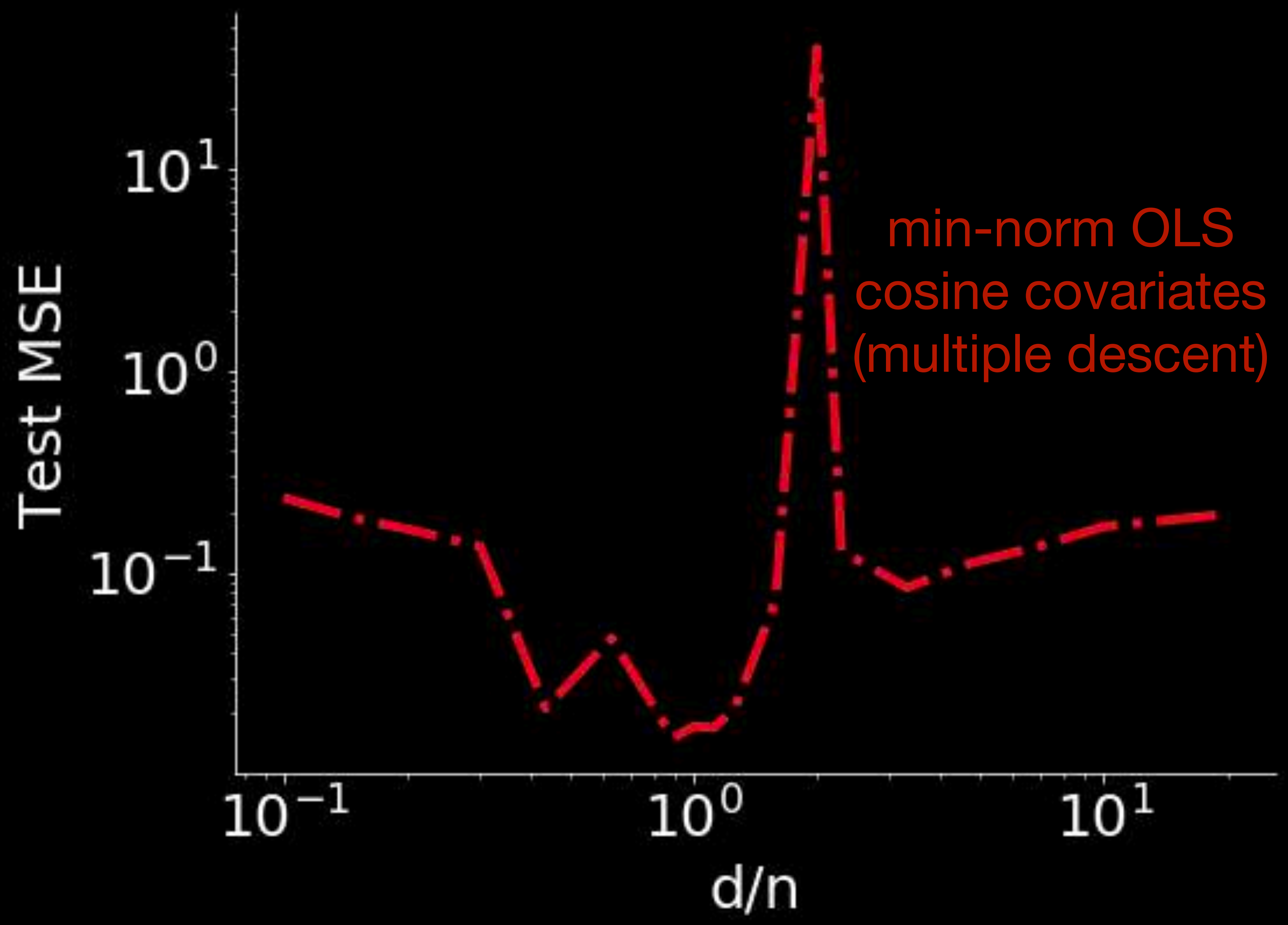

d = number of features
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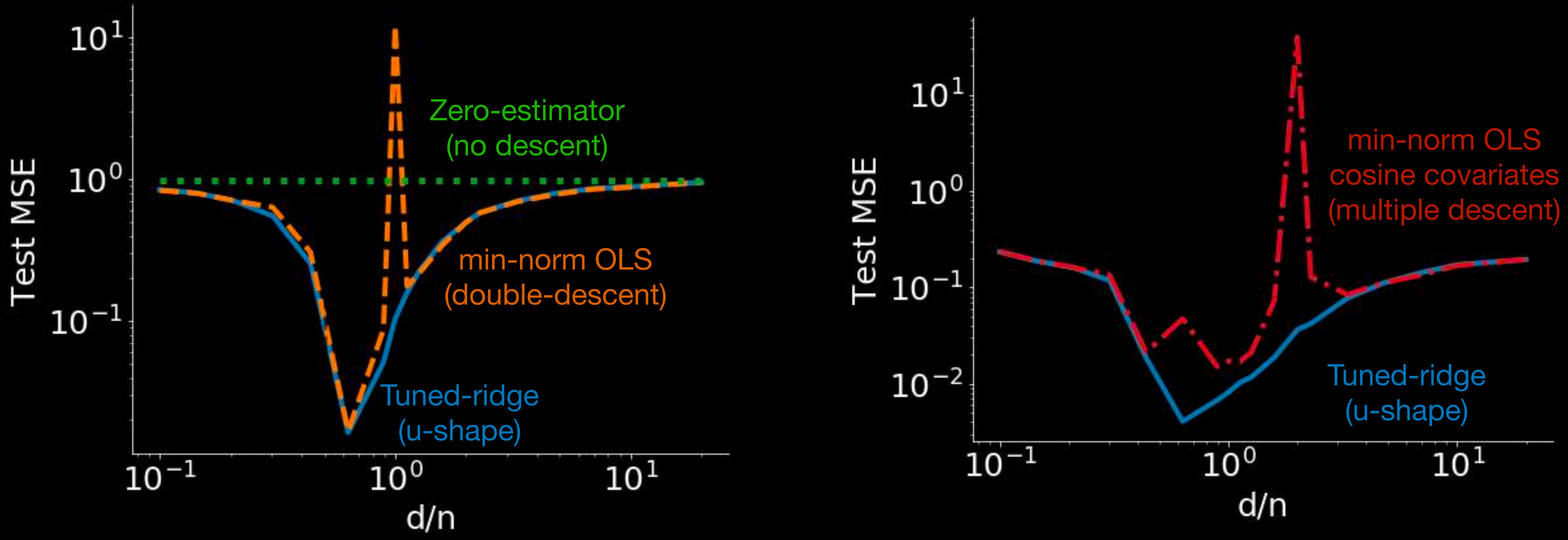
Is double descent a conundrum for the classical wisdom?

We expect the classical U-shaped tradeoff given a **fixed dataset**, and as the "**complexity**" of the fitted estimator varies **in a good estimator class**



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Is double descent a conundrum for the classical wisdom?

We expect the classical U-shaped tradeoff given a **fixed dataset**, and as the "**complexity**" of the fitted estimator varies **in a good estimator class**

Need to pay attention to

- the estimator class, as well as
- the complexity measure

Is parameter counting a valid complexity measure, especially for $d \gg n$?

d = number of features
n = number of samples

Complexity: A tricky concept

A fundamental notion: Kolmogorov's algorithmic complexity

Complexity in Statistics and ML: Useful for model selection

- Test error ~ Train error + Complexity / n^a
- x-axis in bias-variance—often vaguely defined; parameter count often used

n = number of samples

Parameter counting as complexity

Origins for linear regression: $y = X\theta^\star + \varepsilon$

- Akaike Information Criterion (AIC): $d/2$
- Bayesian information criterion (BIC): $\frac{d}{2}\log n$
- Rademacher complexity: $\mathbb{E}\left[\sup_{\theta\in\Theta}\sum \varepsilon_i x_i^\top\theta\right] \sim d$
- Degrees of freedom: trace$(X^\top X) \sim d$
- Vapnik-Chervonenkis dimension: d
- Minimum description length complexity: $\frac{d}{2}\log n$ (asymptotically)

OLS achieves the minimax error of order $\frac{d}{n}$ in low-dimensions $d \ll n$

d = number of features
n = number of samples

but in high-dimensions these complexity measure neither work nor theoretically well-justified

this talk:
a data-dependent complexity using minimum description length that is not just parameter count

Minimum Description Length (MDL)

"Choose the model that gives the shortest description of data"

- Developed by Rissanen with roots in Kolmogorov's algorithmic complexity, also seen as a computable variant based on Shannon's information theory

- **Probability models interpreted as codes:**

  A probability model Q on $\mathscr{Y}$ $\longleftrightarrow$ Encoding observation y with $\log(\frac{1}{Q(y)})$ bits

  Good fit $\longleftrightarrow$ Shorter codelength (description)

- Over the years: Two-stage MDL, mixture MDL, normalized maximum likelihood

Rissanen 76, 80, Barron-Rissanen-Yu 98, Hansen-Yu 02, Grunwald 07

Optimal codes from an MDL perspective

With correctly specified generative model

Two possible objectives

- Minimum expected redundancy

$$\min_q \mathbb{E}_{y\sim p^\star}\left[\log\left(\frac{1}{q(y)}\right) - \log\left(\frac{1}{p^\star(y)}\right)\right]$$

- Minimum worst-case redundancy

$$\min_q \max_y \left[\log\left(\frac{1}{q(y)}\right) - \log\left(\frac{1}{p^\star(y)}\right)\right]$$

Optimal code $q = p^\star$

With unspecified generative model

One objective can be generalized

- Worst-case redundancy w.r.t. a postulated class of codes $\{p_\theta, \theta \in \Theta\}$

$$\min_q \max_y \left[\log\left(\frac{1}{q(y)}\right) - \min_\theta \log\left(\frac{1}{p_\theta(y)}\right)\right]$$

Optimal code: Normalized maximum likelihood (NML)

$$q_{NML}(y) = \frac{\max_\theta p_\theta(y)}{\int \max_{\theta'} p_{\theta'}(z)dz}$$

Rissanen 76, 80, Shtarkov 1981, Barron-Rissanen-Yu 98

NML Complexity = $\int \max_\theta p_\theta(y)dy$

= Worst-case redundancy

= Expected redundancy under known $P^\star$

$\sim \dfrac{d}{2} \log n$ with d-dimensional parametric codes $(d \ll n)$

- However when $\int \max_\theta p_\theta(y)dy = \infty$, the q_{NML} code is not defined.
- E.g., even for the linear model $y = X\theta^\star + \varepsilon$ with Gaussian noise & linear codes:

when $y \in \mathbb{R}^n \implies \int \max_\theta p_\theta(y)dy \propto \int \exp\left(-\frac{1}{2\sigma^2}\|X\hat{\theta}_{OLS} - y\|^2\right)dy = \infty.$

σ^2 = noise (ε) variance

This talk: Tackling the infinity problem of NML

- Prior fixes: Truncate the output space [Barron-Rissanen-Yu 98]
- **This talk**: Regularization + Modified NML complexity
    - In particular, using **ridge regularization** as that allows to obtain best prediction performance across range of models and also enable analytical calculations

Ridge luckiness normalized maximum likelihood

Weight the codes with a luckiness function on parameter space

- **LNML principle:** $\max_\theta p_\theta(y) \leftrightarrow \max_\theta p_\theta(y) w_\theta$ for some ``luckiness function" w_θ
- **Our approach:** Choose luckiness factors $w_{\theta,\Lambda}$ induced by ridge regularization
- For linear models, each $w_{\theta,\Lambda}$ leads to a modified LNML code q_Λ:

$$q_\Lambda(y) \propto \exp\left(-\frac{1}{2\sigma^2}\|X\hat{\theta}_\Lambda - y\|^2 - \frac{1}{2\sigma^2}\hat{\theta}_\Lambda^\top \Lambda \hat{\theta}_\Lambda\right)$$

with $\quad \hat{\theta}_\Lambda = \min_\theta \|X\theta - y\|^2 + \theta^\top \Lambda \theta = (X^\top X + \Lambda)^{-1} X^\top y$

σ^2 = noise variance

Defining the MDL-Complexity

Via the optimal LNML code in a rich ridge class

- To derive complexity: Optimize over Λ—-$\min_{\Lambda} \mathbb{E}_{y \sim p^\star} \left[\log \left(\frac{1}{q_\Lambda(y)} \right) - \log \left(\frac{1}{p^\star(y)} \right) \right] =: R_{opt}$
- Choose a rich class of Λ: $\{UDU^\top, D \succeq 0\}$ with U = eigenvectors($X^\top X$)
- Account codelength for Λ (not present in usual NML):

$$\mathscr{L}(\Lambda) = \sum \log(\lambda_i / \Delta) \text{ for small enough (discretization) } \Delta$$

- Define the MDL-complexity as

$$MDL - COMP = \frac{1}{n}(R_{opt} + \mathscr{L}(\Lambda_{opt})) \text{ where } \Lambda_{opt} \text{ achieves } R_{opt}$$

Main result: Analytical MDL-COMP for linear models

<u>Not</u> just parameter count, instead a function of covariate design & its interaction with signal

If $y \sim \mathcal{N}(X\theta^\star, \sigma^2 I_n)$, and $X^\top X = U\mathrm{diag}(\rho_1, \ldots, \rho_d)U^\top$, $w_i = U^\top\theta^\star$, then

$$R_{opt} = \frac{1}{n}\sum_{i=1}^{\min\{n,d\}} \log\left(1 + \frac{\rho_i w_i^2}{\sigma^2}\right)$$

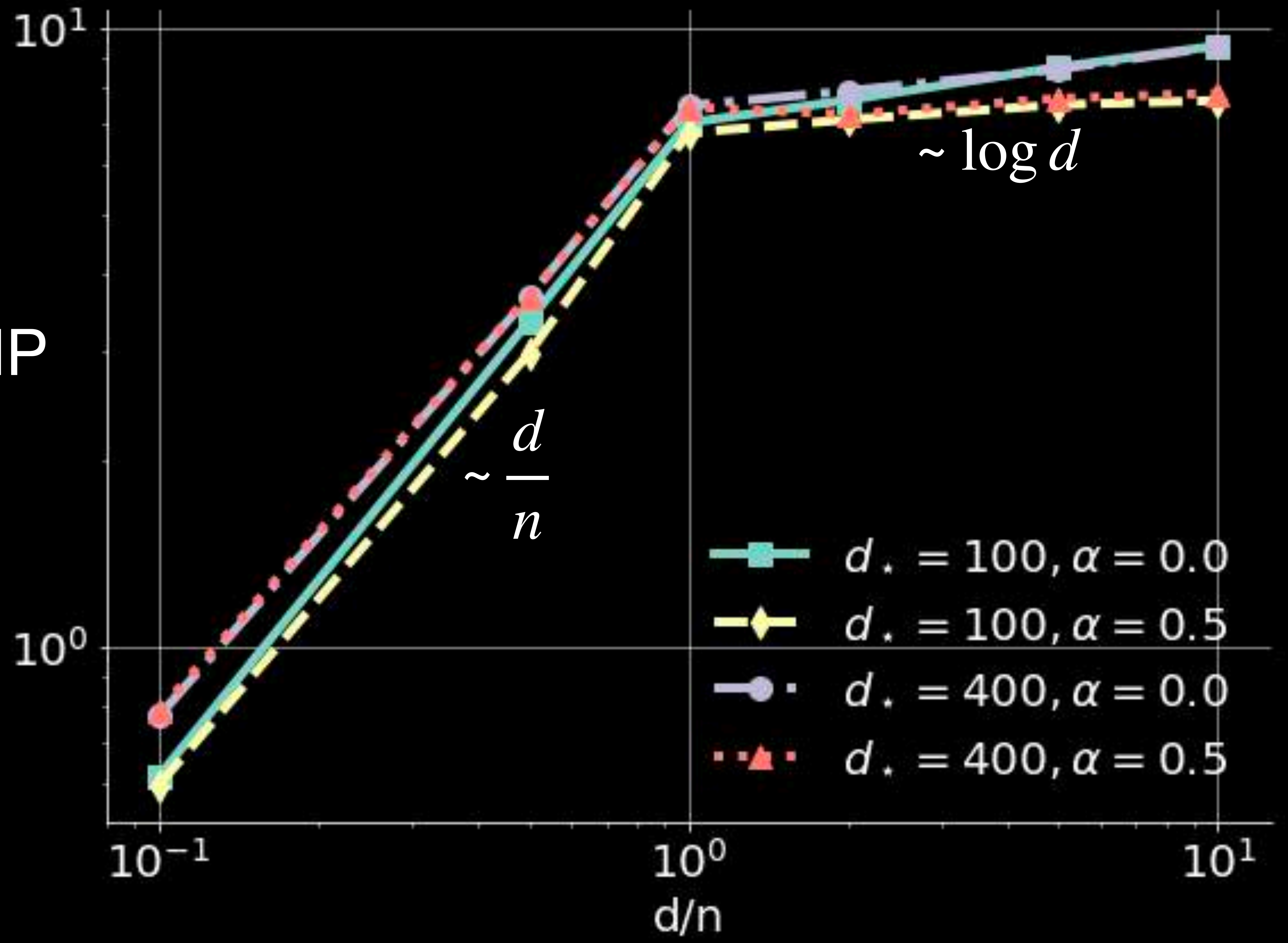
$$MDL - COMP = \frac{1}{n}\sum_{i=1}^{\min\{n,d\}} \log\left(\rho_i + \frac{\sigma^2}{w_i^2}\right) + \min\left\{1, \frac{d}{n}\right\} \log\left(\frac{1}{\Delta}\right)$$

Unpacking the result for Gaussian X

Slow logarithmic growth in overparameterized regime ($d \gg n$)

$n = 200,\ \sigma^2 = 0.1,\ X \sim \mathcal{N}(0, \mathrm{diag}(1, 2^{-\alpha}, \ldots, d^{-\alpha}))$

MDL-COMP



$d_\star$ = true dimensionality

α = eigenvalue decay rate

Other favorable properties about MDL-COMP

The optimal regularization parameter defining linear MDL-COMP also achieves

- **optimal regularization for the in-sample risk** $\min_{\Lambda} \mathbb{E}\left[\sum_{i=1}^{n} (x_i^\top \widehat{\theta}_\Lambda - x_i^\top \theta^\star)^2\right]$
- **best worst-case redundancy over a family of noise distributions**

$$\min_{\Lambda} \max_{P \in \mathscr{P}} \mathbb{E}_{y \sim P} \log\left(\frac{1}{q_\Lambda(y)}\right) \text{ with } \mathscr{P} = \{P \,|\, E_P(y \,|\, X) = X\theta^\star, \mathrm{Var}(y \,|\, X) \preceq \sigma^2 I_n\}$$

Also, MDL-COMP can be **easily extended to kernel methods, where it informs minimax in-sample risk**

Consequences for double descent

Perhaps the issue lies in the estimator

- Since MDL-COMP is monotone in d, using it as the complexity does not change the qualitative nature of the test MSE curves for OLS or ridge
- Double descent likely due to the choice of the estimator, e.g., min-norm OLS
- Conclusion not contradictory with literature on benign overfitting, which provide sufficient conditions for interpolation to generalize well for $d \gg n$ (often estimator and dataset vary *together* with d/n)

… Belkin-Hsu-Ma-Mandal 18, Muthukumar-Vodrahalli-Sahai 19, Hastie-Montanari-Rosset-Tibshirani 19, Tsigler-Bartlett 20, Wu-Xu 20, Nakkiran-Venkat-Kakade-Ma 20 …

Can MDL-COMP be useful for practice?

Let's make it computable from data

$$\text{Prac-MDL-COMP} = \min_{\lambda} \log\left(\frac{1}{q_\lambda(y)}\right)$$

Suggested by our theorems + also consistent with recent suggestions by Grunwald and Roos '20

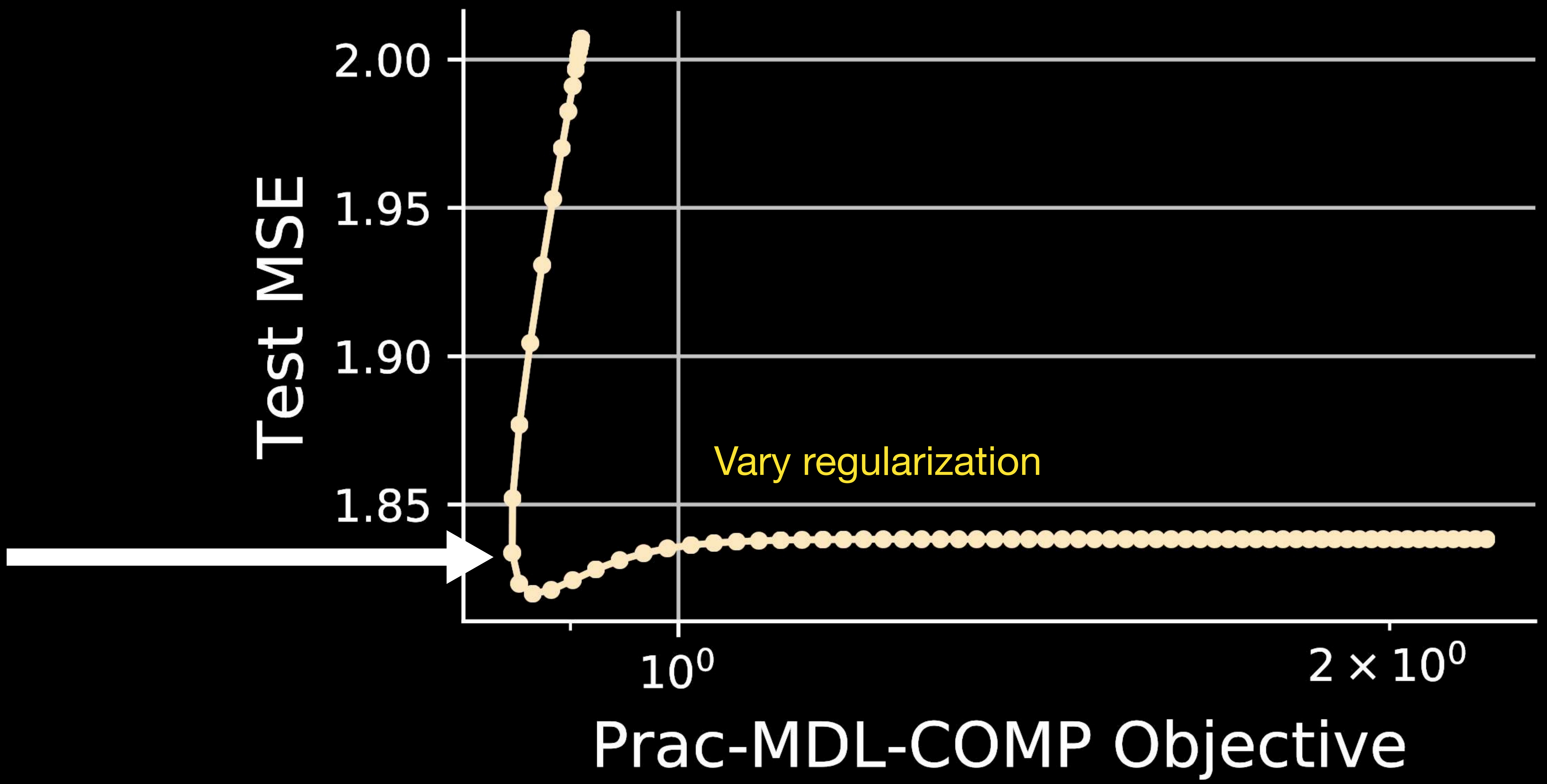
$$= \min_{\lambda}\left[\frac{\|X\hat{\theta}_\lambda - y\|^2}{2\sigma^2} + \frac{\lambda\|\hat{\theta}_\lambda\|^2}{2\sigma^2} + \boxed{\sum_{i=1}^{\min\{n,d\}} \log\left(1+\frac{\rho_i}{\lambda}\right)}\right]$$

where

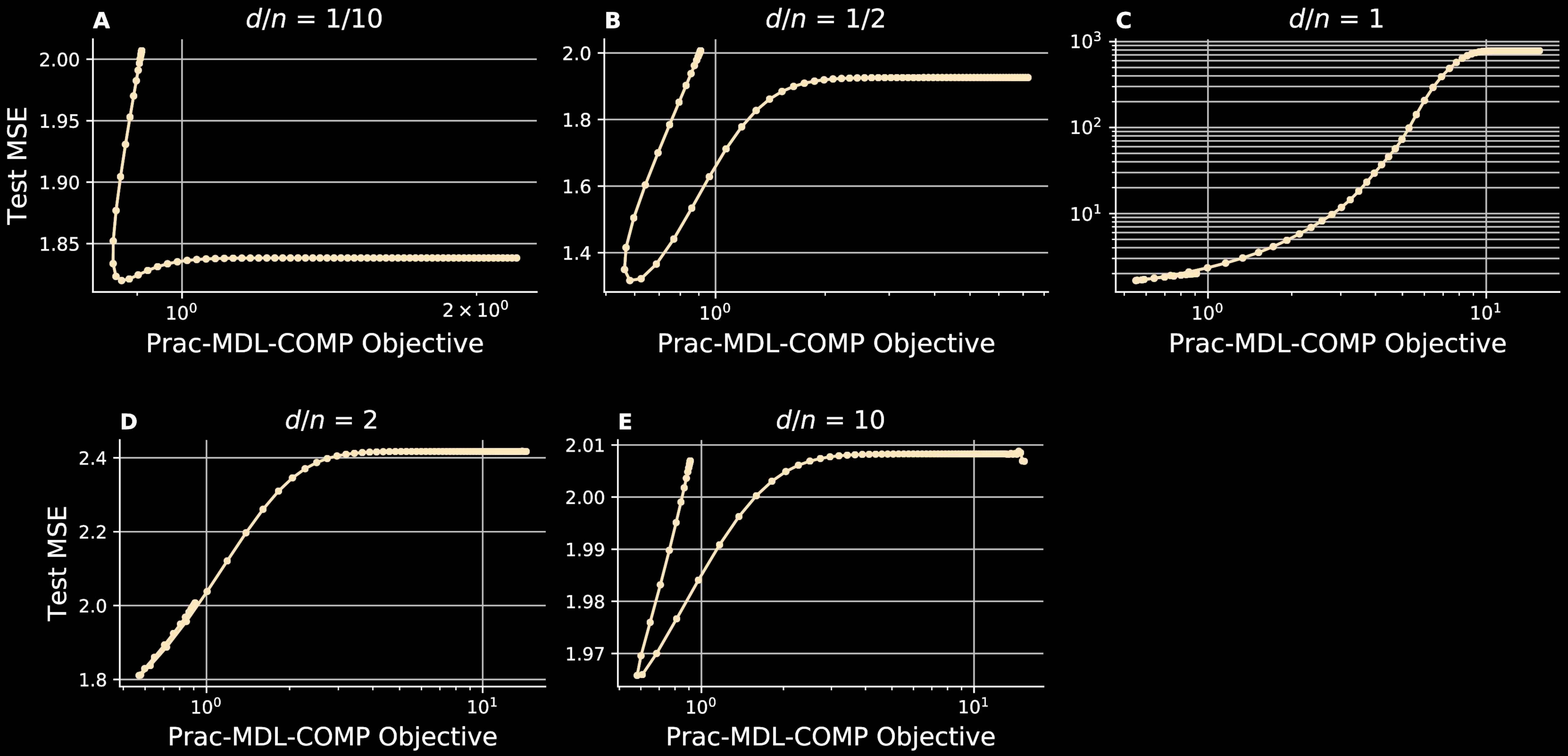
$\hat{\theta}_\lambda = (X^\top X + \lambda I)^{-1} X^\top y$ and ρ_i denote the eigenvalues of $X^\top X$

Model selection with Prac-MDL-COMP

Test MSE minimizer close to the minimizer of Prac-MDL-COMP objective

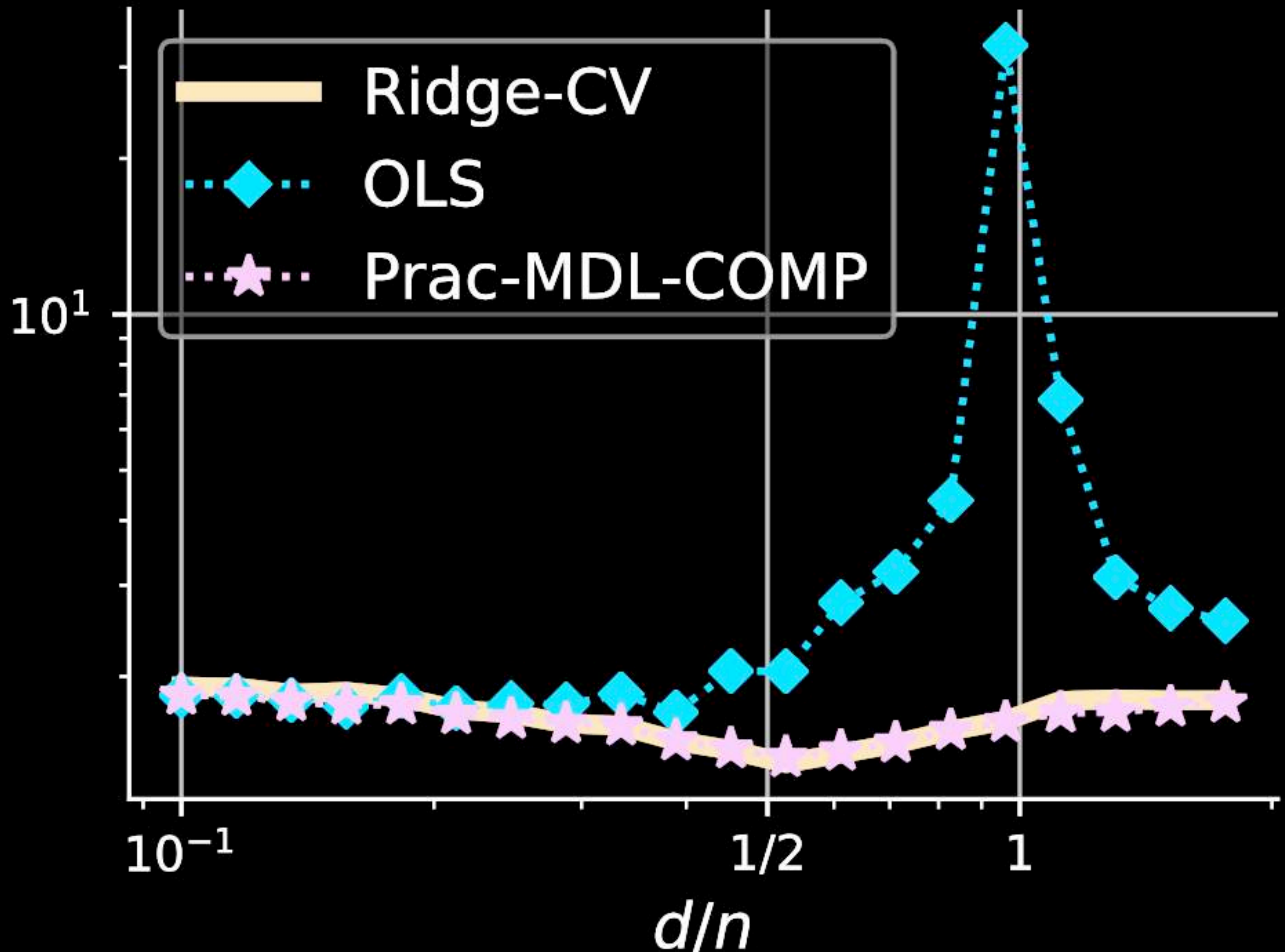


Model selection with Prac-MDL-COMP



Prac-MDL-COMP removes the double descent

Test performance competitive compared to cross-validation



Using Prac-MDL-COMP for hyperparameter tuning

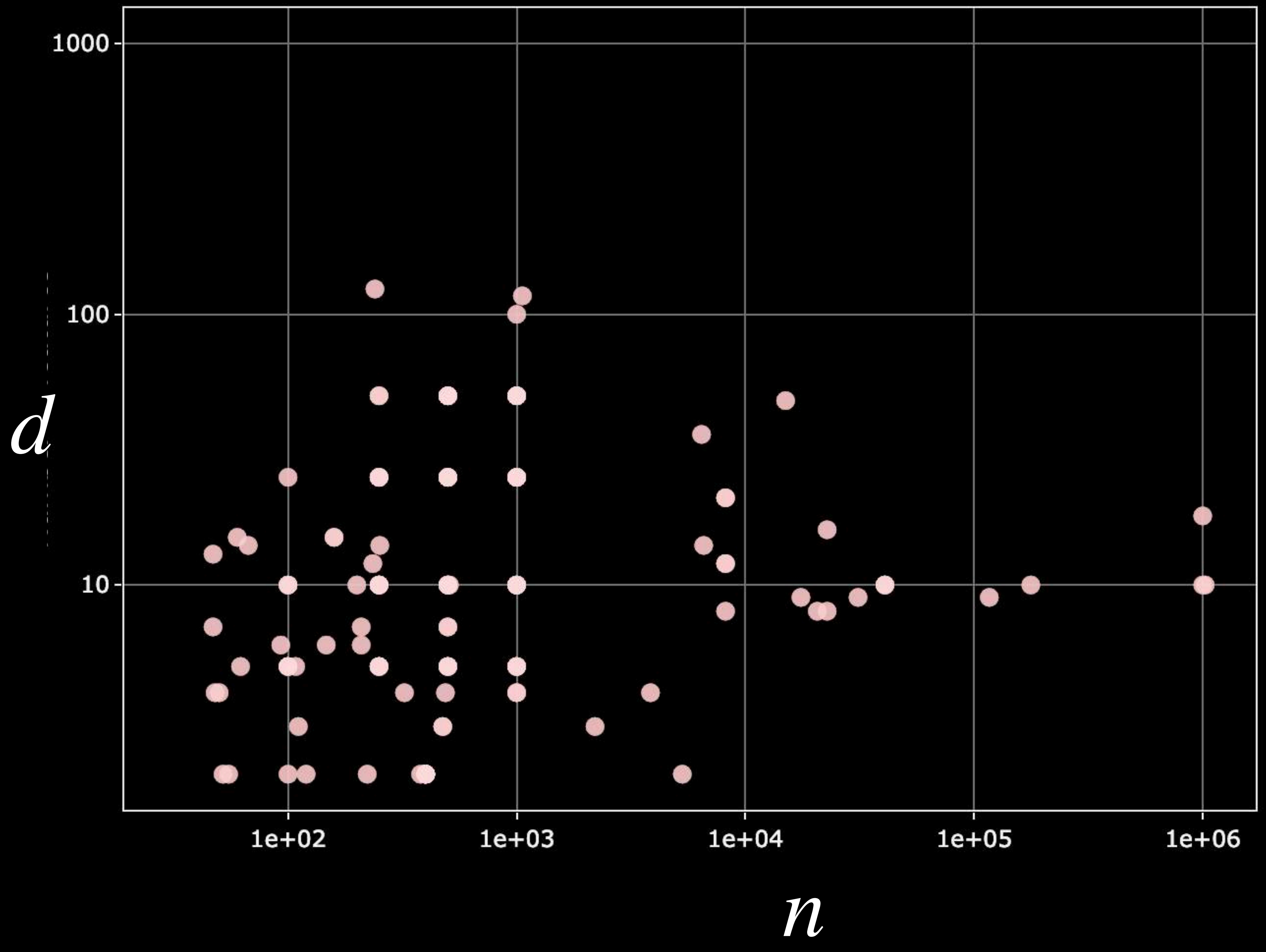
$$\min_{\lambda} \left[\frac{\|X\widehat{\theta}_\lambda - y\|^2}{2\sigma^2} + \frac{\lambda \|\widehat{\theta}_\lambda\|^2}{2\sigma^2} + \sum_{i=1}^{\min\{n,d\}} \log\left(1 + \frac{\rho_i}{\lambda}\right) \right]$$

K-fold computational savings compared to K-fold cross validation (CV)

Experiments on PMLB datasets

Diverse set of tabular datasets

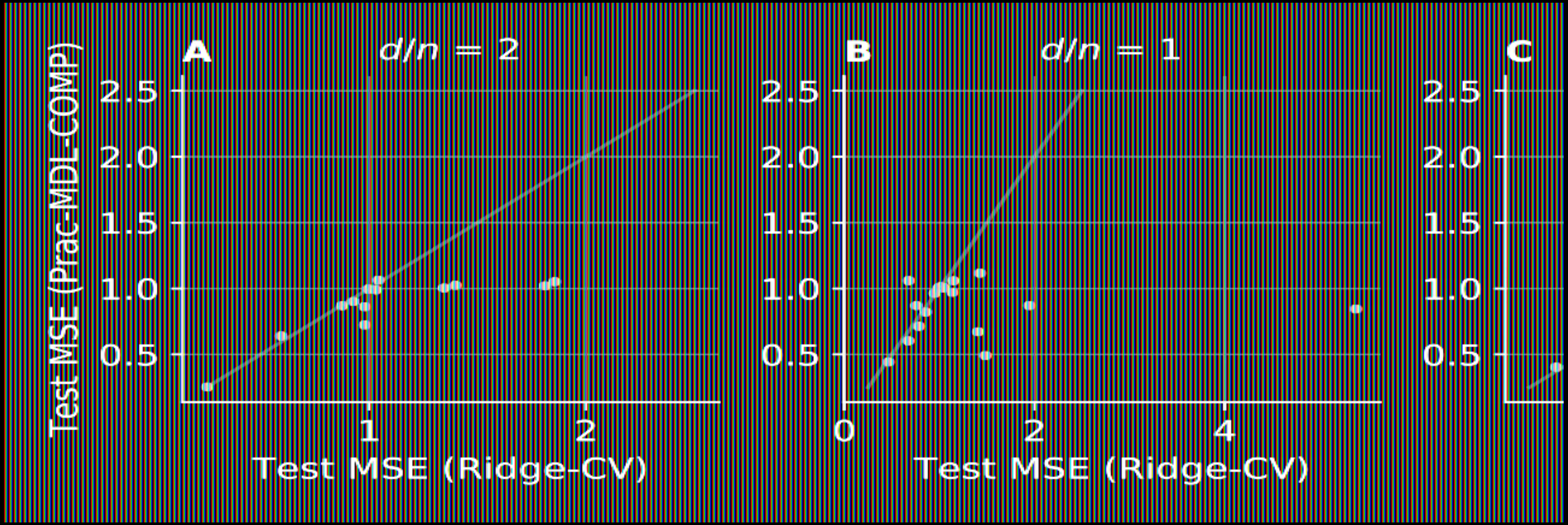
- Predicting breast cancer from image features
- Predicting automobile prices
- Election results from previous elections



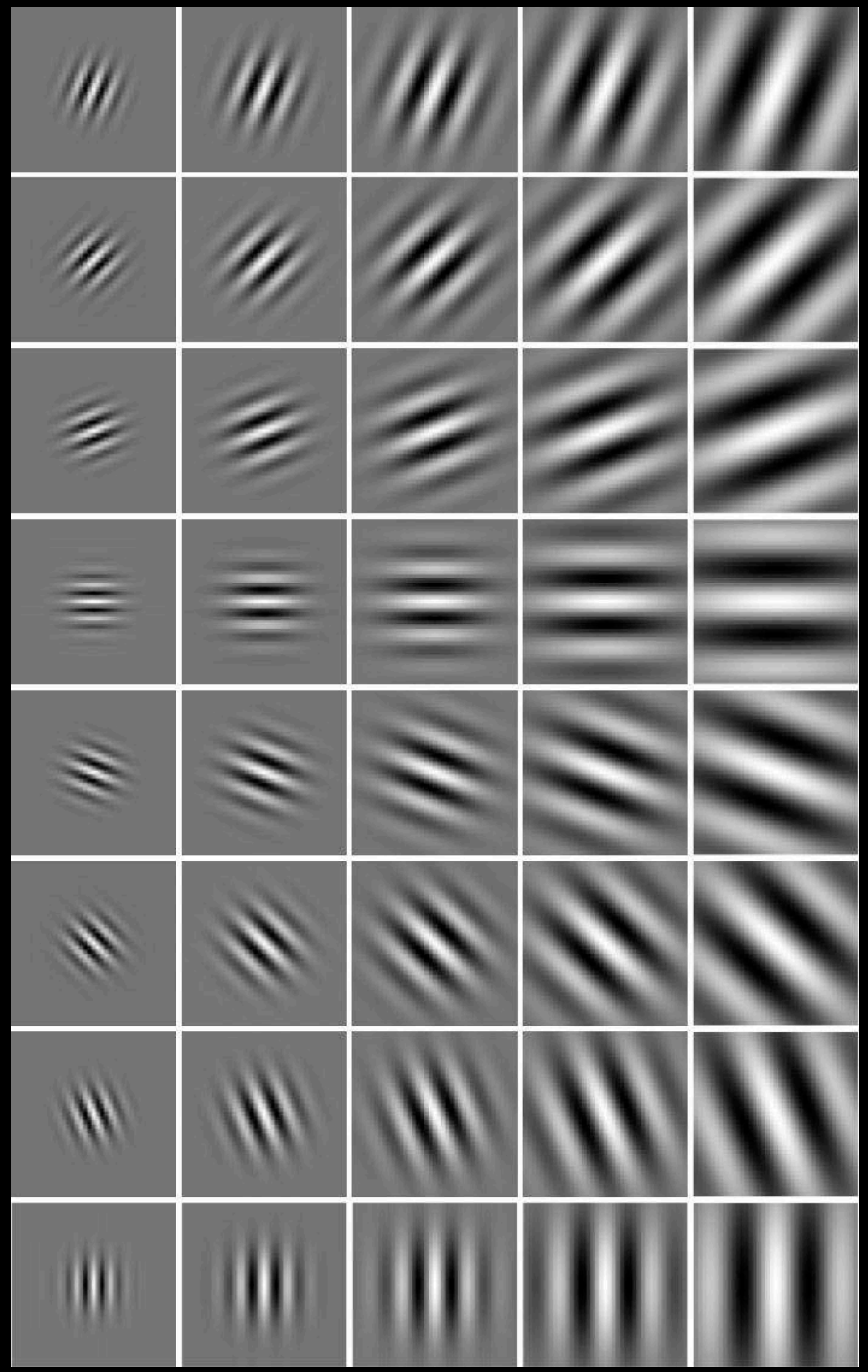
PMLB: a large benchmark suite for machine learning evaluation and comparison
Olson-Cava-Orzechowski-Urbanowicz-Moore 17

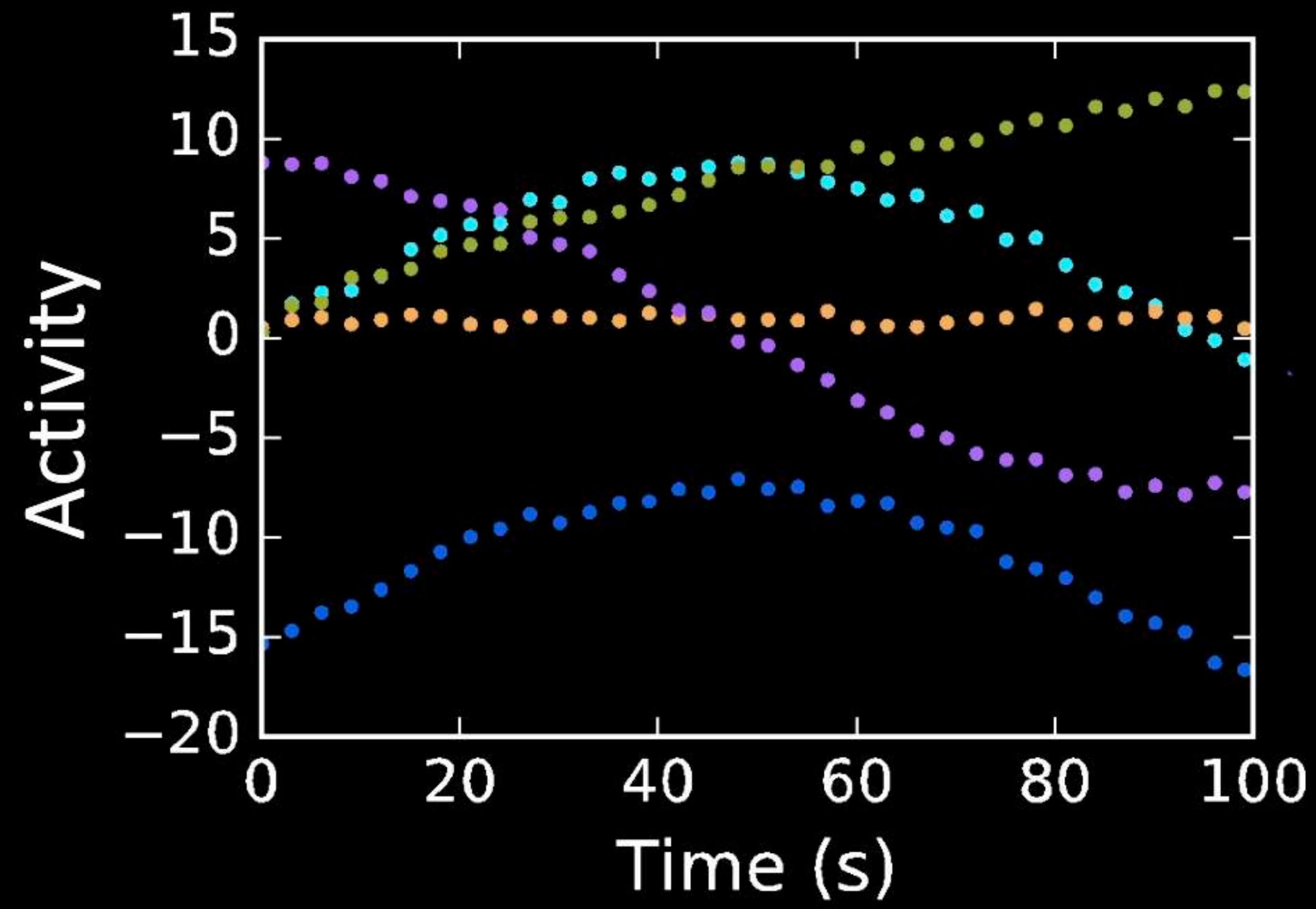
Experiments on PMLB datasets

MDL-COMP better for hyper-parameter tuning in low-data settings



fMRI experimental setup





Video clip → Extract gabor features → Predictive model → fMRI voxel responses

Nishimoto-Vu-Naselaris-Benjamini-Yu-Gallant 11

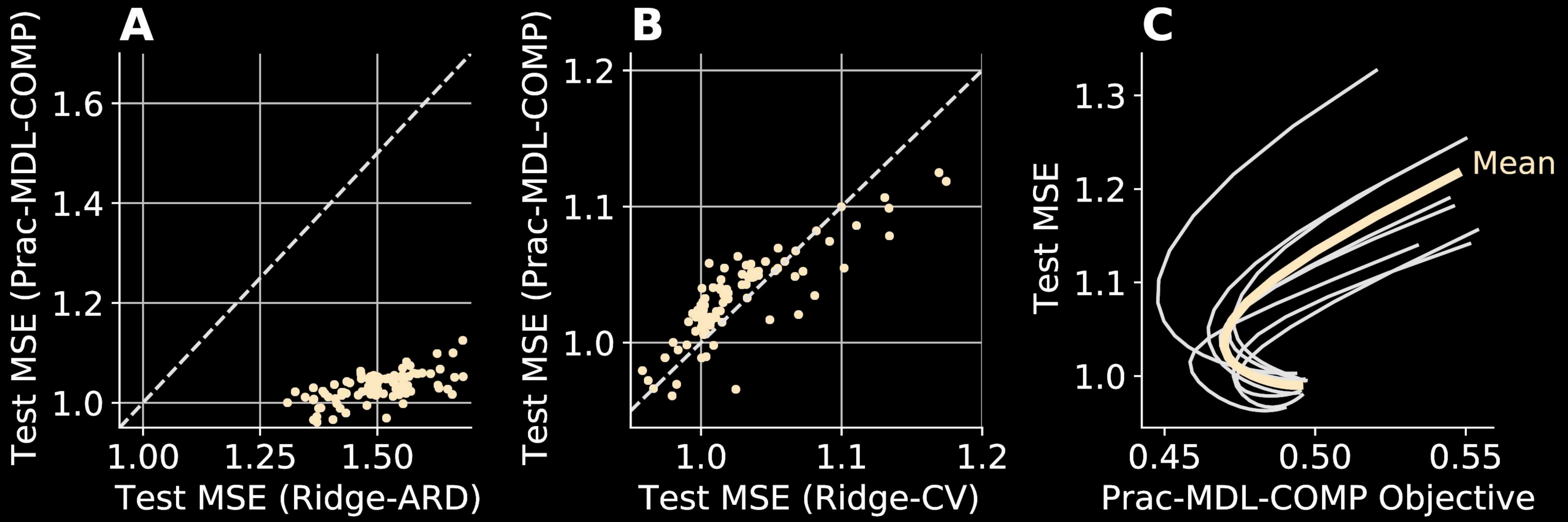
d = 1280

n_train = 7200

n_test= 540

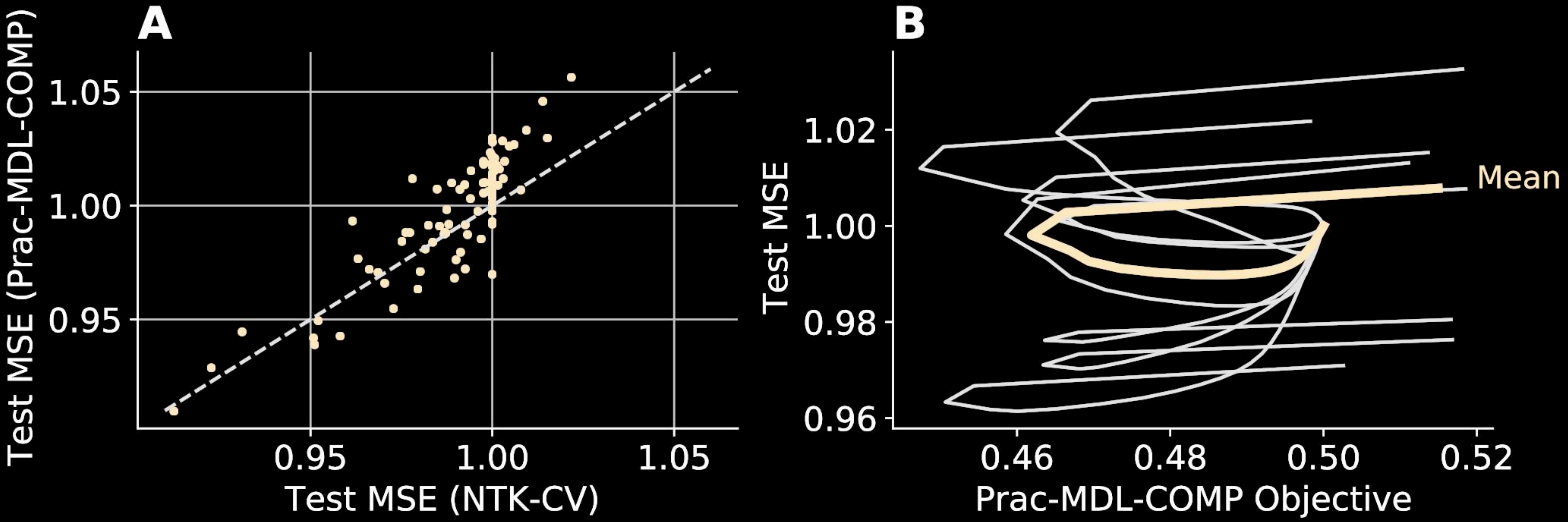
Experiments on fMRI data from 100 voxels

MDL-COMP better than Bayesian-ARD regression, and pretty comparable to CV tuning



Experiments on neural tangent kernels

(2 layer RELU neural tangent kernel)



Once again, MDL-COMP pretty comparable to CV tuning

Summary

MDL-COMP—a modified NML complexity measure using optimal ridge estimators

- Not just parameter count—$\log d$ scaling for $d \gg n$ with Gaussian covariates
- Hints that double descent likely due to choice of estimator
- Provides competitive-to-CV but computationally-better hyper-parameter tuning
- Open questions:

  Analytical relations between MDL-COMP and out-of-sample generalization?

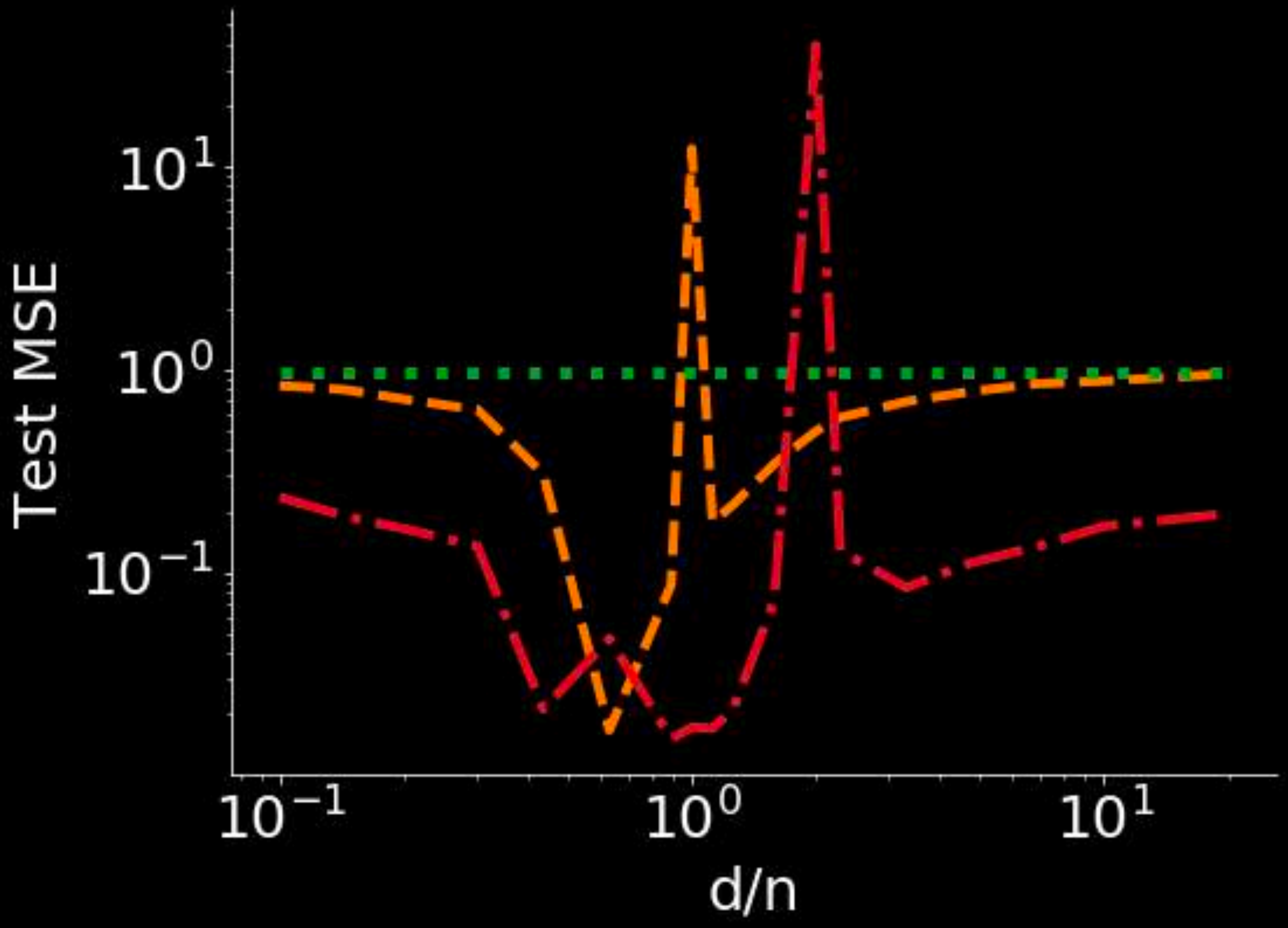
  MDL-COMP for classification + complex models like neural networks?

https://rzrsk.github.io

Additional slides

Bias-variance tradeoff: Few things to note..

- We should expect a tradeoff *given*
  - some fixed data
  - as the "complexity" of the fitted estimator changes
- Do not expect a tradeoff for
  - poor choice of estimators
  - poor choice of complexity



MDL-COMP for kernel methods

Universal codes induced by kernel ridge regression

- Define the code Q_λ:

$$q_\lambda(y) \propto \exp\left(-\frac{1}{2\sigma^2}\|K\widehat{\theta}_\lambda - y\|^2 - \frac{\lambda}{2\sigma^2}\widehat{\theta}_\lambda^\top K\widehat{\theta}_\lambda\right)$$

where

$$\widehat{\theta}_\lambda = \min_\theta \|K\theta - y\|^2 + \lambda\theta^\top K\theta = (K + \lambda I)^{-1}y$$

- This choice comes from kernel ridge regression:

$$\min_{f \in \mathscr{H}} \sum_{i=1}^{n} (f(x_i) - y_i)^2 + \lambda\|f\|_{\mathscr{H}}^2$$

Kernel ridge regression

- One can show that for the optimization proboem

$$\min_{f \in \mathscr{H}} \sum_{i=1}^{n} (f(x_i) - y_i)^2 + \lambda \|f\|_{\mathscr{H}}^2,$$

it suffices to consider the functions of the form

$$f = \sum_{i=1}^{n} \theta_i K(x_i, \cdot\,),$$

and this leads to the kernel ridge regression problem in the previous slide

MDL-COMP for kernel regression

- Let ρ_i denote the eigenvalues of the kernel matrix $(K(x_i, x_j))_{i,j=1}^n$ and suppose $y \sim \mathcal{N}(f^\star(X), \sigma^2 I_n)$ for some $f^\star$ in RKHS of K, then

$$\mathscr{R}_{opt} \leq \frac{1}{2n}\left[\min_{\lambda} \frac{\lambda \|f^\star\|_{\mathscr{H}}^2}{\sigma^2} + \sum_{i=1}^{n} \log\left(1 + \frac{\rho_i}{\lambda}\right)\right]$$

(no easy closed-form)

- Since there is only a single hyper-parameter, we can directly take

$$MDL - COMP = \mathscr{R}_{opt}$$

Unpacking MDL-COMP for Sobolev kernels

- For Sobolev kernel of smoothness α, the eigenvalues decay like $\rho_i \sim i^{-2\alpha}$, and one can derive

$$\mathcal{R}_{opt} \leq C \left(\frac{\|f^\star\|_{\mathcal{H}}^2}{\sigma^2} \right)^{\frac{1}{2\alpha+1}} \cdot n^{-\frac{2\alpha}{2\alpha+1}}$$

Neural tangent kernels (NTK)

NTK approximates neural net with infinite width

Jacot et al. 2018

- Varies with number of layers and nonlinearity

  - $K(x, x') = \mathbb{E}_{\theta \sim W}\left[\left\langle \frac{\partial f(\theta, x)}{\partial \theta}, \frac{\partial f(\theta, x')}{\partial \theta} \right\rangle\right]$

- Analytical expressions for simple architectures
  (e.g., cosine kernel for 2 layer Relu networks)

- Software libraries for computing the kernel for deeper networks

Kernel version of the computation

$$\text{Prac-MDL-COMP} = \min_{\lambda} \log\left(\frac{1}{q_\lambda(y)}\right)$$

$$= \min_{\lambda}\left[\frac{\|K\widehat{\theta}_\lambda - y\|^2}{2\sigma^2} + \frac{\lambda\widehat{\theta}_\lambda^\top K\widehat{\theta}_\lambda}{2\sigma^2} + \sum_{i=1}^{n}\log\left(1+\frac{\rho_i}{\lambda}\right)\right]$$

where

$\widehat{\theta}_\lambda = (K+\lambda I)^{-1}y$ and ρ_i denote the eigenvalues of the kernel matrix K

Proofs

Proof sketch for linear models

$$
\begin{aligned}
\mathcal{D}_{\mathrm{KL}}(\mathbb{P}_{\theta_\star} \,\|\, \mathbb{Q}_{\mathbf{\Lambda}}) &= \mathbb{E}_{\mathbf{y}}\left[\log \frac{p(\mathbf{y};\mathbf{X},\theta_\star)}{q_{\mathbf{\Lambda}}(\mathbf{y})}\right] \\
&= \mathbb{E}_{\mathbf{y}}\left[\log\left(\frac{\frac{1}{(2\pi\sigma^2)^{n/2}}\exp\left(-\frac{1}{2\sigma^2}\|\mathbf{y}-\mathbf{X}\theta_\star\|^2\right)}{\frac{1}{\mathrm{C}_{\mathbf{\Lambda}}(2\pi\sigma^2)^{n/2}}\exp\left(-\frac{1}{2\sigma^2}\|\mathbf{y}-\mathbf{X}\widehat{\theta}\|^2-\frac{1}{2\sigma^2}\widehat{\theta}^\top\mathbf{\Lambda}\widehat{\theta}\right)}\right)\right] \\
&= -\underbrace{\mathbb{E}_{\mathbf{y}}\left[\frac{1}{2\sigma^2}\|\mathbf{y}-\mathbf{X}\theta_\star\|^2\right]}_{=:T_1} + \underbrace{\mathbb{E}\left[\frac{1}{2\sigma^2}\|\mathbf{y}-\mathbf{X}\widehat{\theta}\|^2+\frac{1}{2\sigma^2}\widehat{\theta}^\top\mathbf{\Lambda}\widehat{\theta}\right]}_{=:T_2} + \underbrace{\log \mathrm{C}_{\mathbf{\Lambda}}}_{=:T_3}. \qquad (31)
\end{aligned}
$$

$$T_2 = \frac{(n - \min\{n,d\})}{2} + \frac{1}{2} \sum_{i=1}^{\min\{n,d\}} \frac{(\rho_i w_i^2/\sigma^2 + 1)\lambda_i}{\lambda_i + \rho_i}, \quad \text{and} \tag{33a}$$

$$T_3 = \frac{1}{2} \sum_{i=1}^{\min\{n,d\}} \log\left(\frac{\rho_i + \lambda_i}{\lambda_i}\right) \tag{33b}$$

$$\frac{1}{n}\mathcal{D}_{\mathrm{KL}}(\mathbb{P}_{\theta_\star} \,\|\, \mathbb{Q}_{\mathbf{\Lambda}}) = T_1 + T_2 + T_3$$

$$= -\frac{\min\{n,d\}}{2n} + \frac{1}{2n}\sum_{i=1}^{\min\{n,d\}} \underbrace{\left(\frac{(\rho_i w_i^2/\sigma^2 + 1)\lambda_i}{\lambda_i + \rho_i} + \log\left(\frac{\rho_i + \lambda_i}{\lambda_i}\right)\right)}_{=: f_i(\lambda_i)}. \tag{34}$$

Finally to compute the $\mathcal{R}_{\text{opt}}$ (32), we need to minimize the KL-divergence (34) where we note the objective depends merely on $\lambda_1, \ldots, \lambda_{\min\{n,d\}}$. We note that the objective (RHS of equation (34)) is separable in each term λ_i. We have

$$f_i'(\lambda_i) = 0 \quad \Longleftrightarrow \quad -\frac{(\rho_i w_i^2/\sigma^2 + 1)}{(1 + \rho_i/\lambda_i)^2} + \frac{1}{1 + \rho_i/\lambda_i} = 0 \quad \Longleftrightarrow \quad \lambda_i^{\text{opt}} = \frac{\sigma^2}{w_i^2}. \tag{35}$$

Proof sketch for the result with Gaussian X

- When $X \in \mathbb{R}^{n \times d}$ has i.i.d. $\mathcal{N}(0,1/n)$ entries, then for $X^\top X = U\text{diag}(\rho_1, \ldots, \rho_d)U^\top$
    - The matrix U has uniform distribution over the set of $d \times d$ orthonormal matrices and hence for any fixed $\theta^\star$, the coordinates of $w = U^\top \theta^\star$ are identically distributed, and we can use the approximation $w_i^2 \approx \dfrac{\|\theta^\star\|^2}{d}$

Proof sketch for the result with Gaussian X

- When $X \in \mathbb{R}^{n\times d}$ has i.i.d. $\mathcal{N}(0,1/n)$ entries, then for $X^\top X = U\text{diag}(\rho_1, \ldots, \rho_d)U^\top$
    - The eigenvalues ρ_i follow Marcenko-Pastur Law with the following approximation
    - $d \ll n, \quad X^\top X \approx I_d, \quad \rho_i \approx 1$
    - $d > n, \quad X^\top X \approx \begin{bmatrix} \frac{d}{n} I_n & 0 \\ 0 & 0 \end{bmatrix}, \quad \rho_i \begin{cases} \approx \frac{d}{n}, & i \leq n \\ = 0, & i > n \end{cases}$

Marcenko-Pastur 67, Silverstein 95, Tulino-Verdu 04

Two-stage MDL

Two-stage MDL

- Consider a parametric class of codes $\{p_\theta, \theta \in \Theta\}$, and then use the valid codelength for any fixed p_θ

$$\log\left(\frac{1}{p_\theta(y)}\right)$$

- Minimizing this codelength is same as MLE over the given parametric class

- But the choice of $\widehat{\theta}$ varies with y, so need to account for the codelength needed to transmit the value of $\widehat{\theta}$

Two-stage MDL

- Thus the overall codelength is

$$\boxed{\log\left(\frac{1}{p_{\hat{\theta}}(y)}\right)} + \boxed{\frac{d}{2}\log n}$$

Codelength for data

Codelength for d-dimensional parameter upto $1/\sqrt{n}$ resolution

- For a fixed parametric class, same as MLE (since the second term is constant)
- For a family of parametric classes, same as BIC procedure (model selection)

MDL-COMP vs Cross-validation

- For $n \times d$ covariates, for each value of λ, the computational costs are
  - **K-fold cross-validation**: K x OLS solver = $K \times (nd^2 + \min(n^3, d^3))$
  - **Prac-MDL-COMP**: 1 x SVD solver = $nd^2 + n^2 d$

Prac-MDL-COMP provides a proxy for complexity and saves K-fold computation!

Issues with NML

Issues with NML: Linear model

- Then Q_{NML} is given by

$$q_{NML}(y) \propto \max_{\theta} p_{\theta}(y) = p_{\hat{\theta}}(y) = \frac{1}{(2\pi\sigma^2)^{n/2}} \exp\left(-\frac{1}{2\sigma^2}\|X\hat{\theta} - y\|^2\right)$$

$$\hat{\theta} = \arg\max p_{\theta}(y) = \arg\min_{\theta} \|X\theta - y\|^2 = \hat{\theta}_{OLS}$$

(We can use min-norm OLS when $d > n$)

Issues with NML: Linear model

- If $\mathscr{Y}$ is not compact (even when d<n)

$$\int \frac{1}{(2\pi\sigma^2)^{n/2}} \exp\left(-\frac{1}{2\sigma^2}\|X\widehat{\theta} - y\|^2\right) dy = \infty$$

- Easiest to see when $d > n$ so that $X\widehat{\theta} = y$, and we have

$$\int \frac{1}{(2\pi\sigma^2)^{n/2}} \exp\left(-\frac{1}{2\sigma^2}\|X\widehat{\theta} - y\|^2\right) dy = \int_{\mathbb{R}^n} \frac{1}{(2\pi\sigma^2)^{n/2}} dy = \infty$$

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Optimal code: With known true model $P^\star$ is $P^\star$

- When $y \sim P^\star$, the expected code-length when using code Q is given by

$$\mathbb{E}_{y \sim P^\star} \log \left(\frac{1}{Q(y)} \right) = \mathbb{KL}(P^\star \| Q) + H(P^\star)$$

- Minimized when $Q = P^\star$, since redundancy is non-negative
- $P^\star$ also minimizes the worst-case regret

$$p^\star = \arg\min_q \max_y \left[\log \left(\frac{1}{q(y)} \right) - \log \left(\frac{1}{p^\star(y)} \right) \right] \text{ such that } \int q(z) dz \leq 1$$

Expressions

Unpacking the result for Gaussian X

Slow logarithmic growth in overparameterized regime ($d \gg n$)

- When $X \in \mathbb{R}^{n \times d}$ has i.i.d. $\mathcal{N}(0, 1/n)$ entries, then

$$\text{MDL-COMP} \approx \begin{cases} \frac{d}{n}\log\left(1+\frac{d_\star}{r^2}\right)+\frac{d}{n}\log\left(\frac{1}{\Delta}\right), & \text{if } d \in [1, d_\star] \\ \frac{d}{n}\log\left(1+\frac{d}{r^2}\right)+\frac{d}{n}\log\left(\frac{1}{\Delta}\right), & \text{if } d \in [d_\star, n] \\ \log\left(\frac{d}{n}+\frac{d}{r^2}\right)+\log\left(\frac{1}{\Delta}\right), & \text{if } d \in [n, \infty) \end{cases}$$

[here $d_\star$ denotes the true dimensionality of $\theta^\star$, and we assume $\mathbb{E}[y \mid X] = \tilde{X}\theta^\star$ where $\tilde{X}$ denotes the first $d_\star$ columns of X; and $r^2 = \|\theta^\star\|^2$]

MDL-COMP scaling for other designs

Numerical computation: Another example

$$n = 200,\ \sigma^2 = 0.1,\ X \sim \mathcal{N}(0, \begin{bmatrix} 16\mathbf{I}_s & 0 \\ 0 & \mathbf{I}_{d-s} \end{bmatrix})$$

MDL-COMP