DOUBLE TROUBLE IN DOUBLE DESCENT

BIAS AND VARIANCE(S) IN THE LAZY REGIME

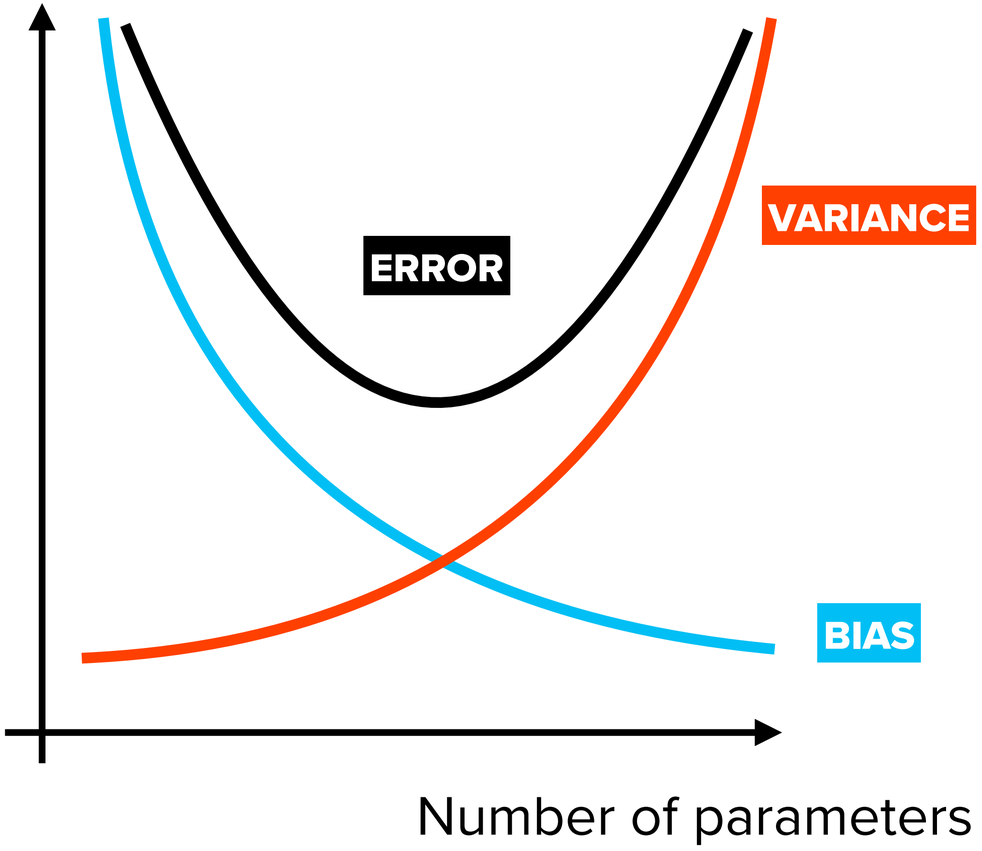
STÉPHANE D'ASCOLI, MARIA REFINETTI,
GIULIO BIROLI, FLORENT KRZAKALA

ÉCOLE NORMALE SUPÉRIEURE DE PARIS

FROM CLASSICAL THEORY

BIAS-VARIANCE TRADEOFF

"The price to pay for achieving low bias is high variance"
(Geman et al., 1992)



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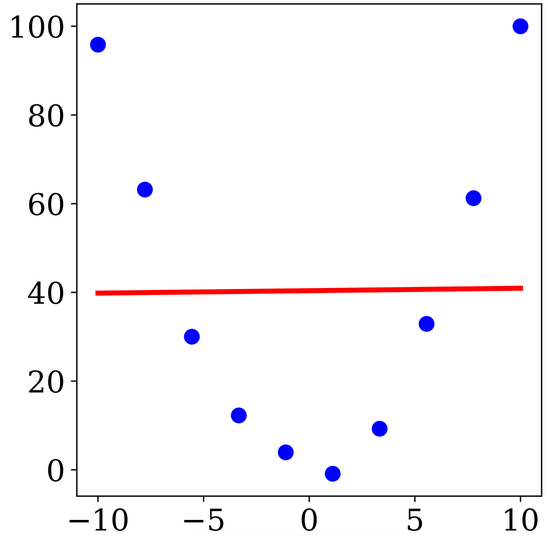
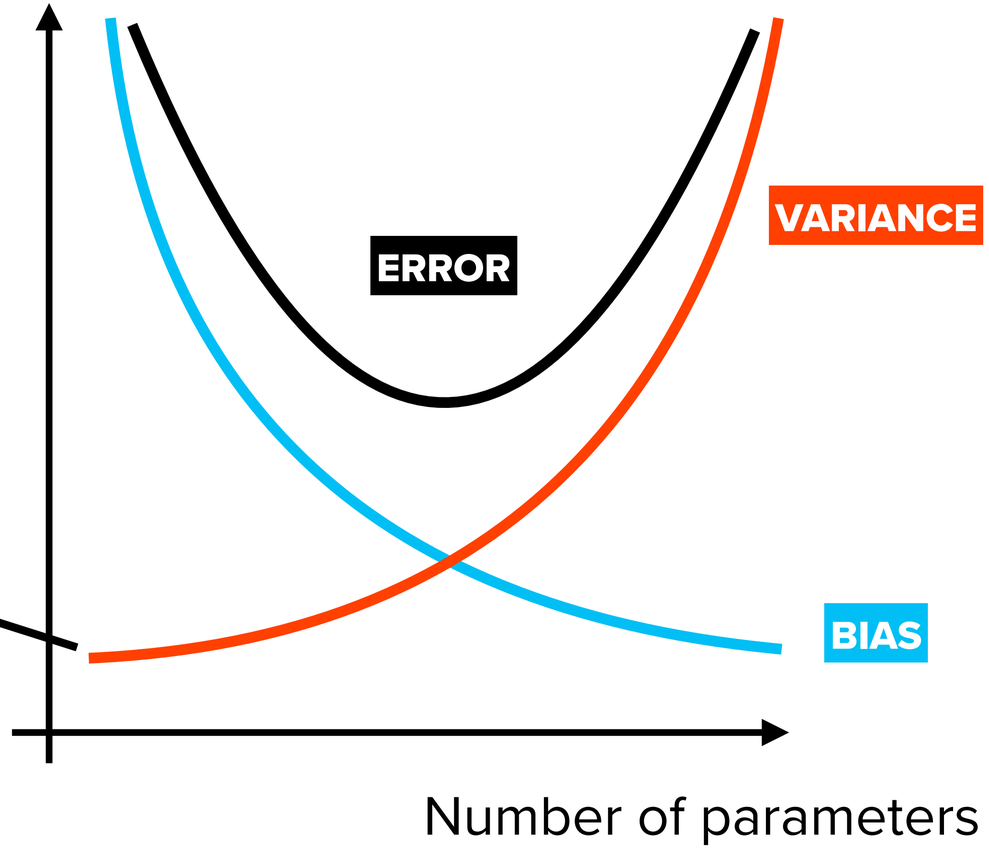
TOO FEW PARAMETERS:
HIGH BIAS, LOW VARIANCE



UNDERFIT



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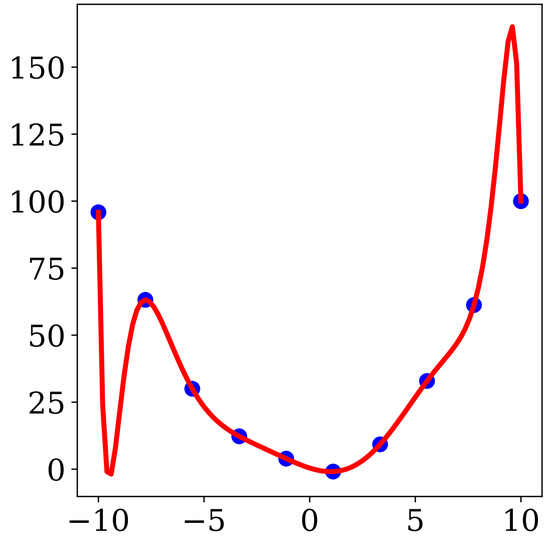
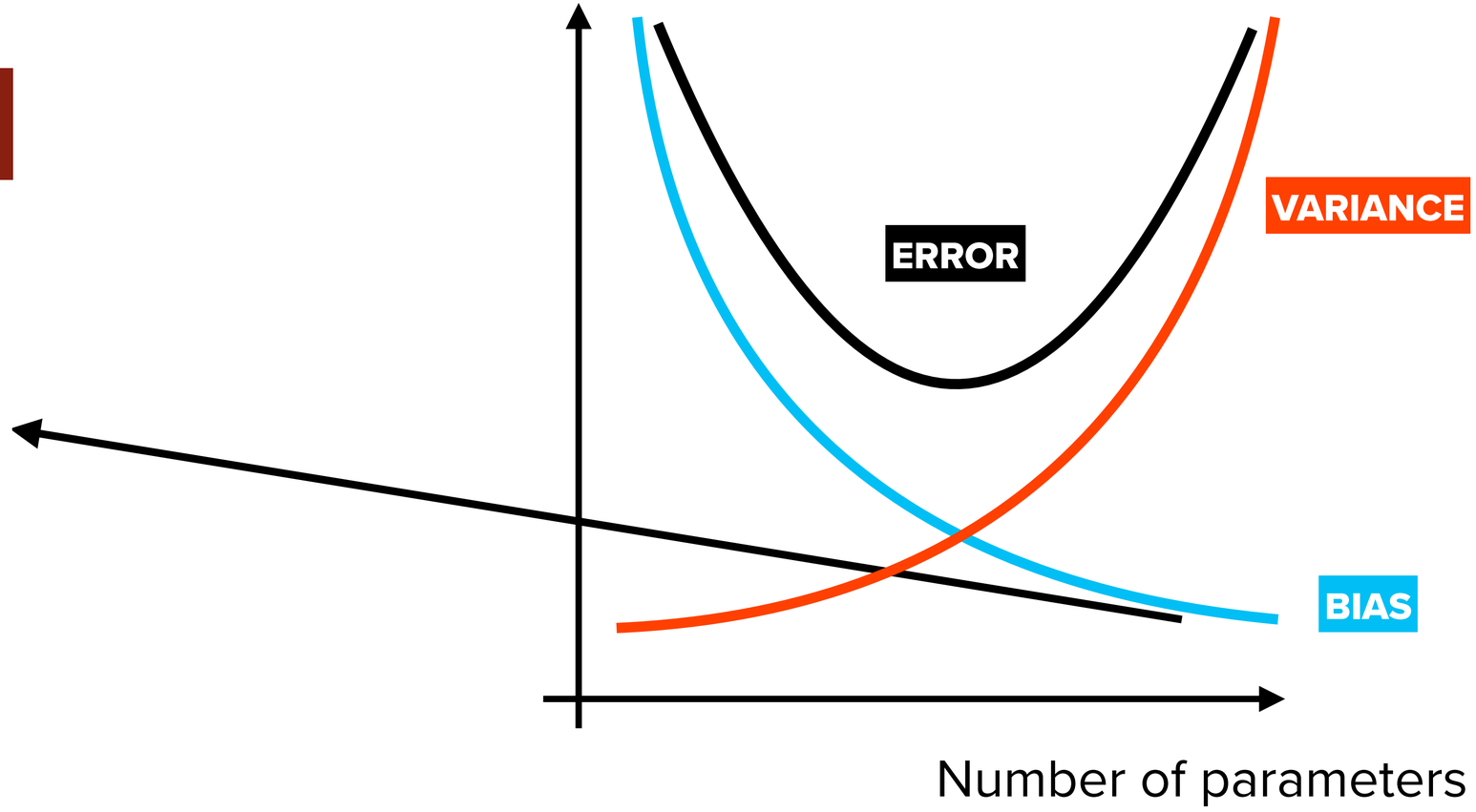
TOO MANY PARAMETERS: LOW BIAS, HIGH VARIANCE



OVERFIT



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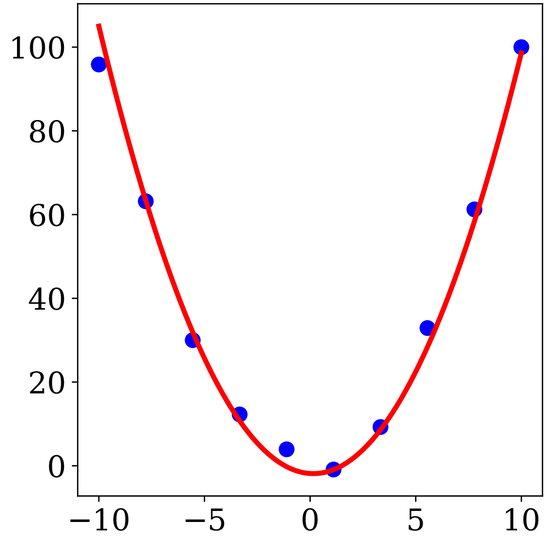
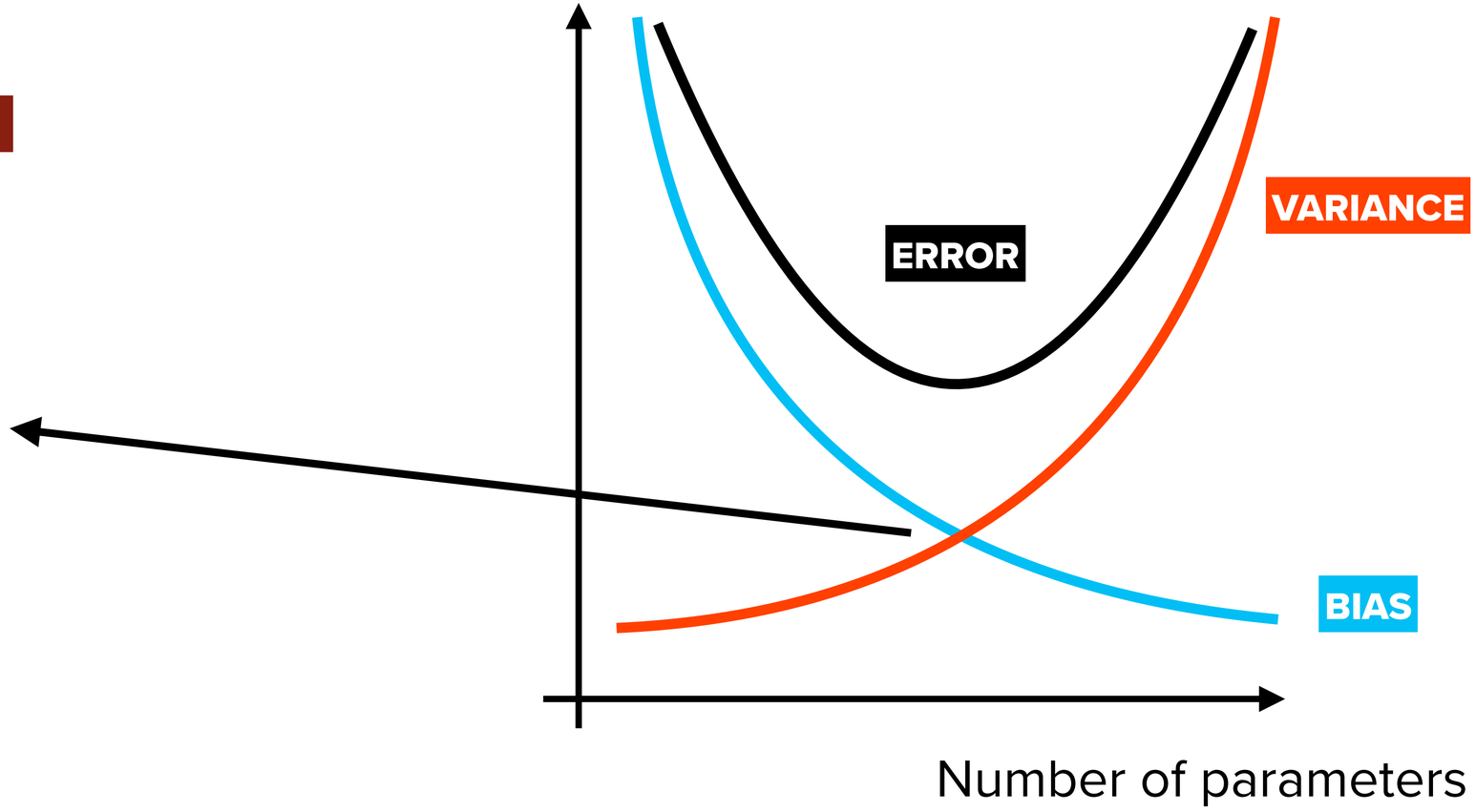
BALANCED





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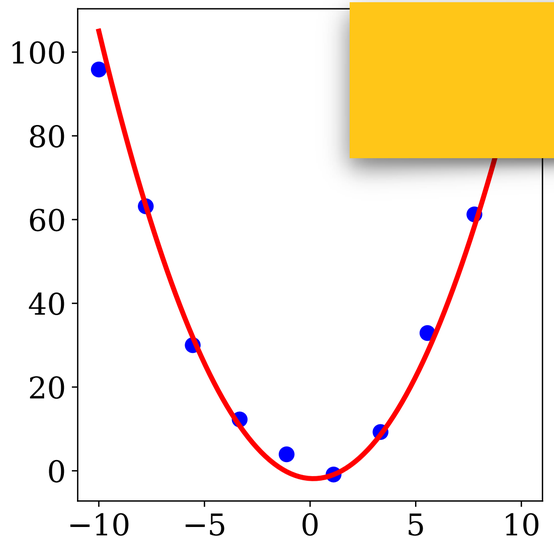
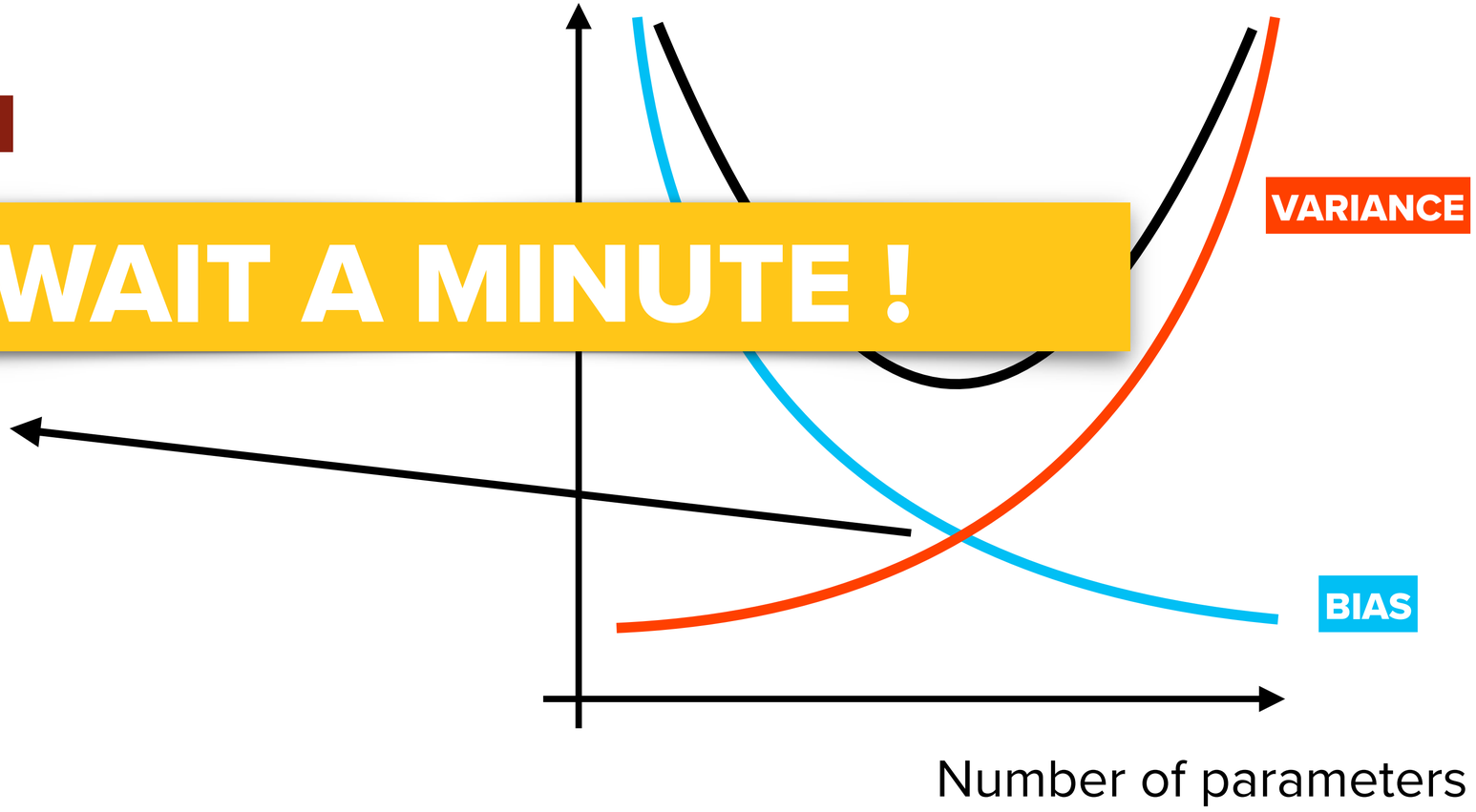
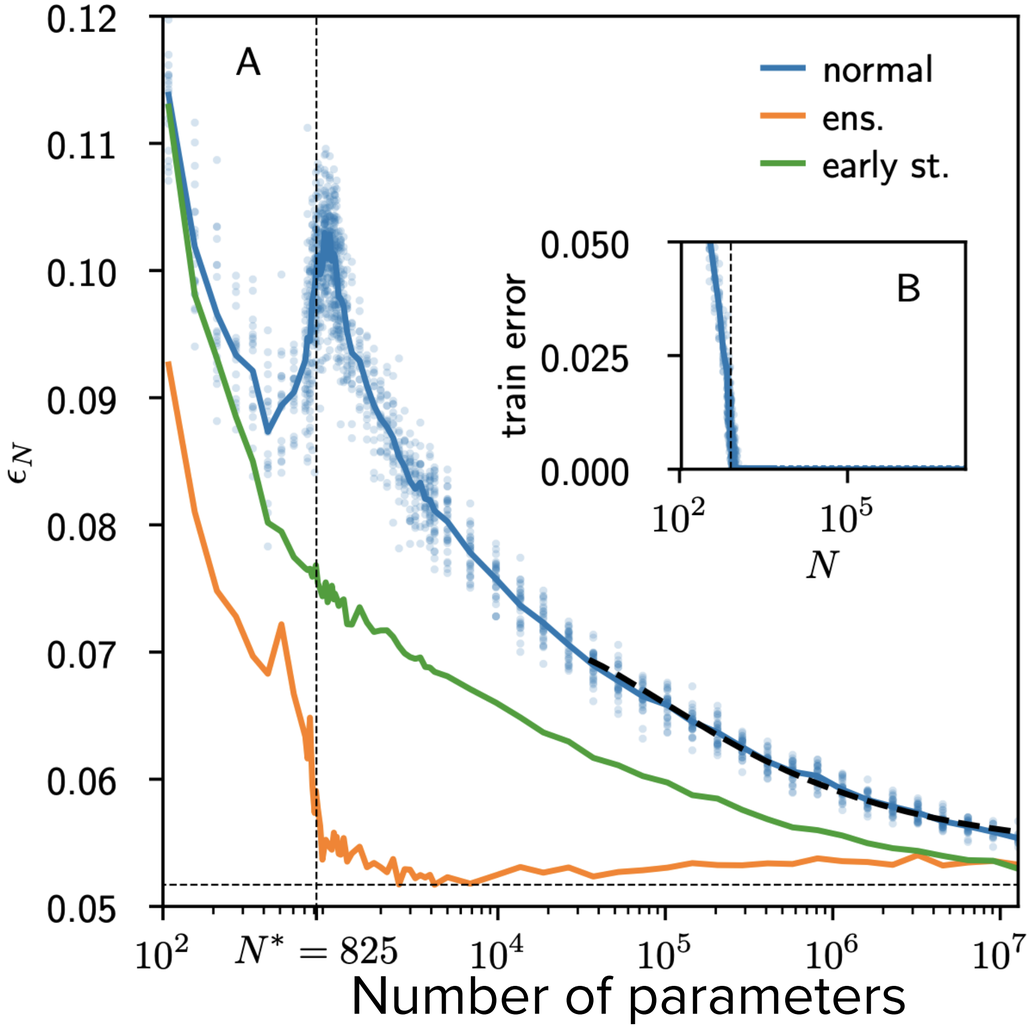


WAIT A MINUTE !



TO DOUBLE DESCENT



See also

Belkin et al. 2019

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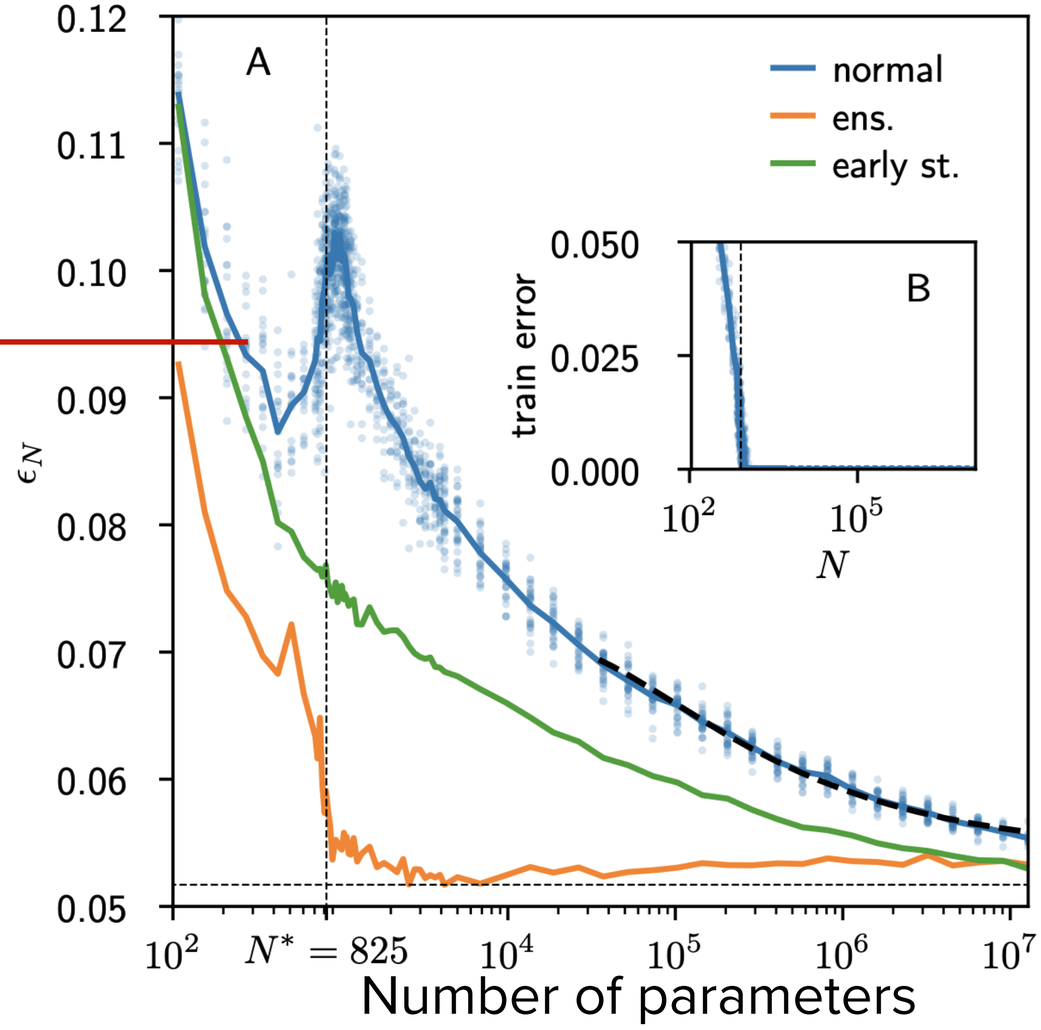
TO DOUBLE DESCENT

"U" shaped curve in the underparametrized regime



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Peak in Test Error
At interpolation threshold

"U" shaped curve in the
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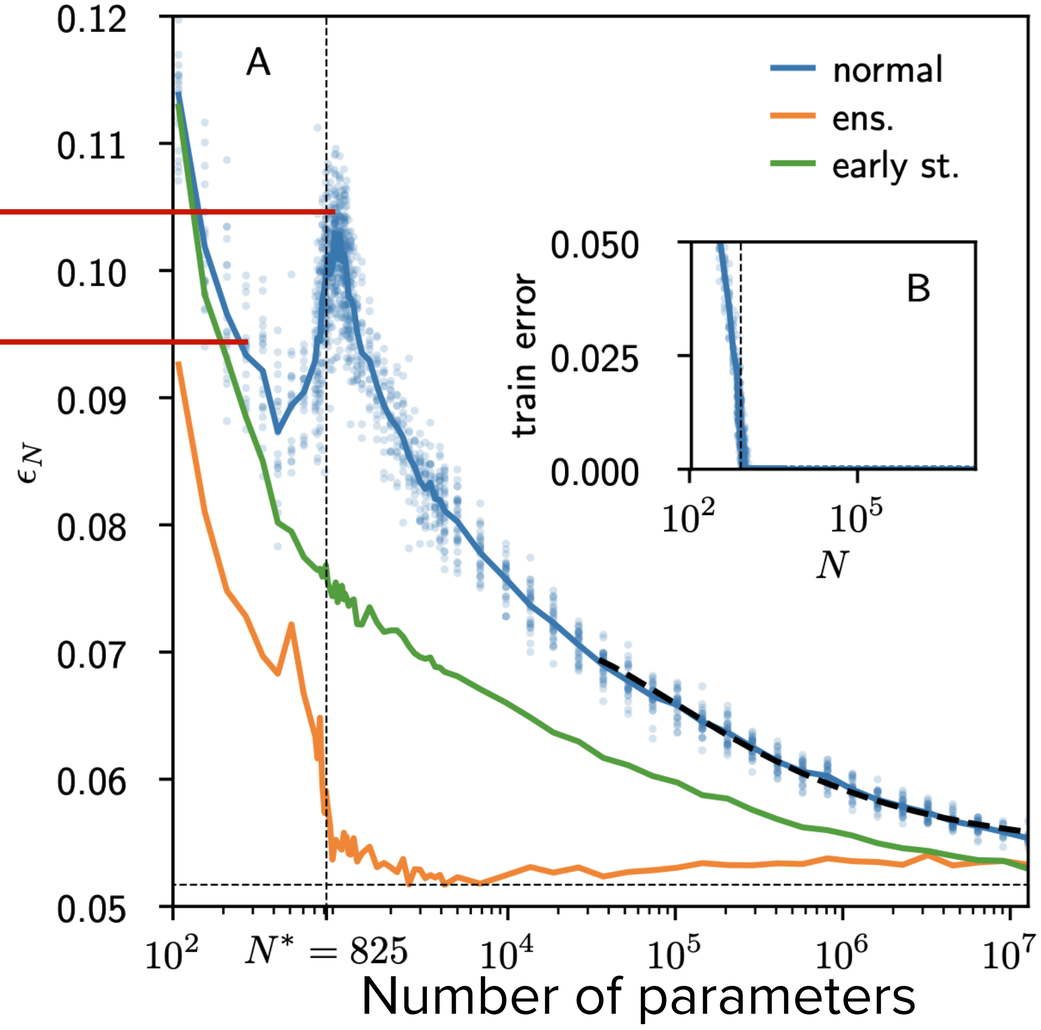

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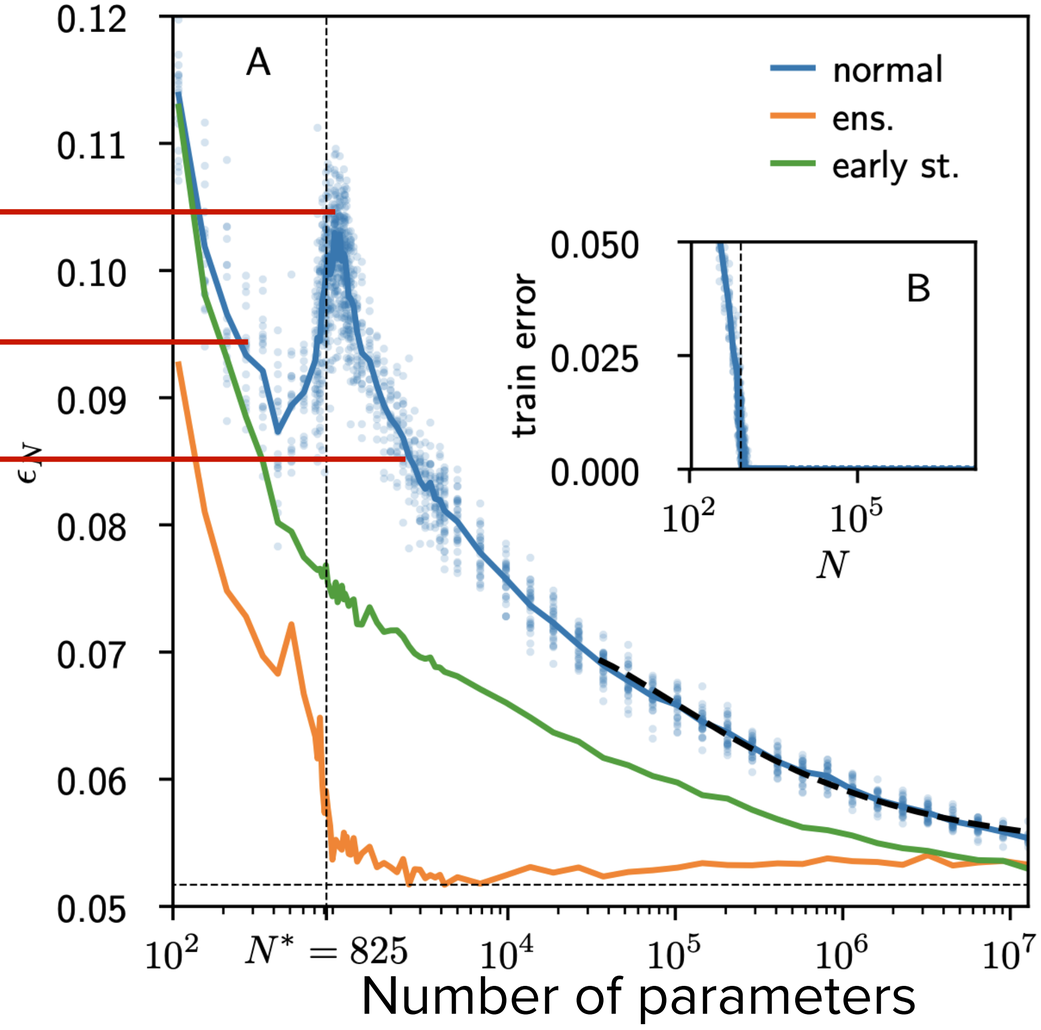
Monotonous decrease in the overparametrized regime



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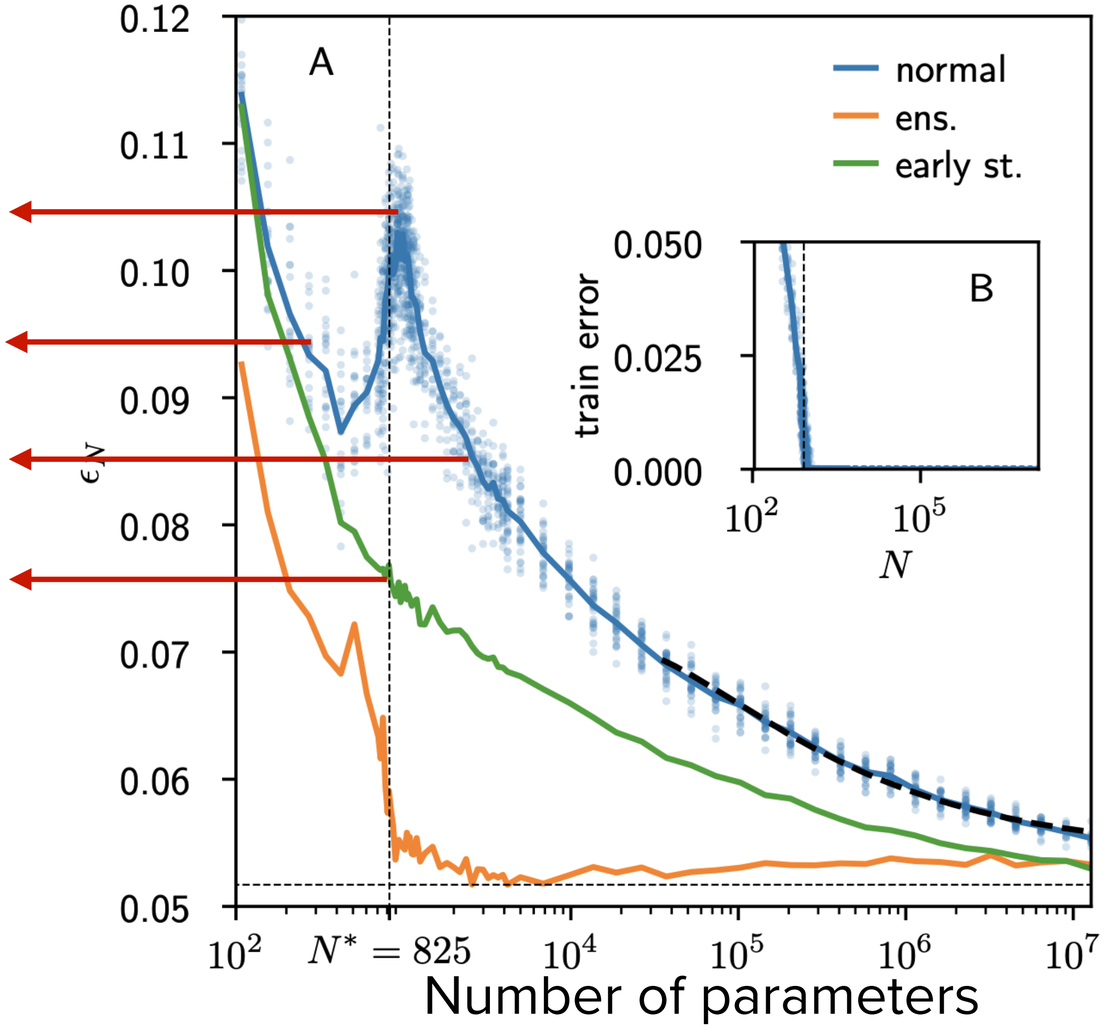
Peak suppressed by **regularisation**



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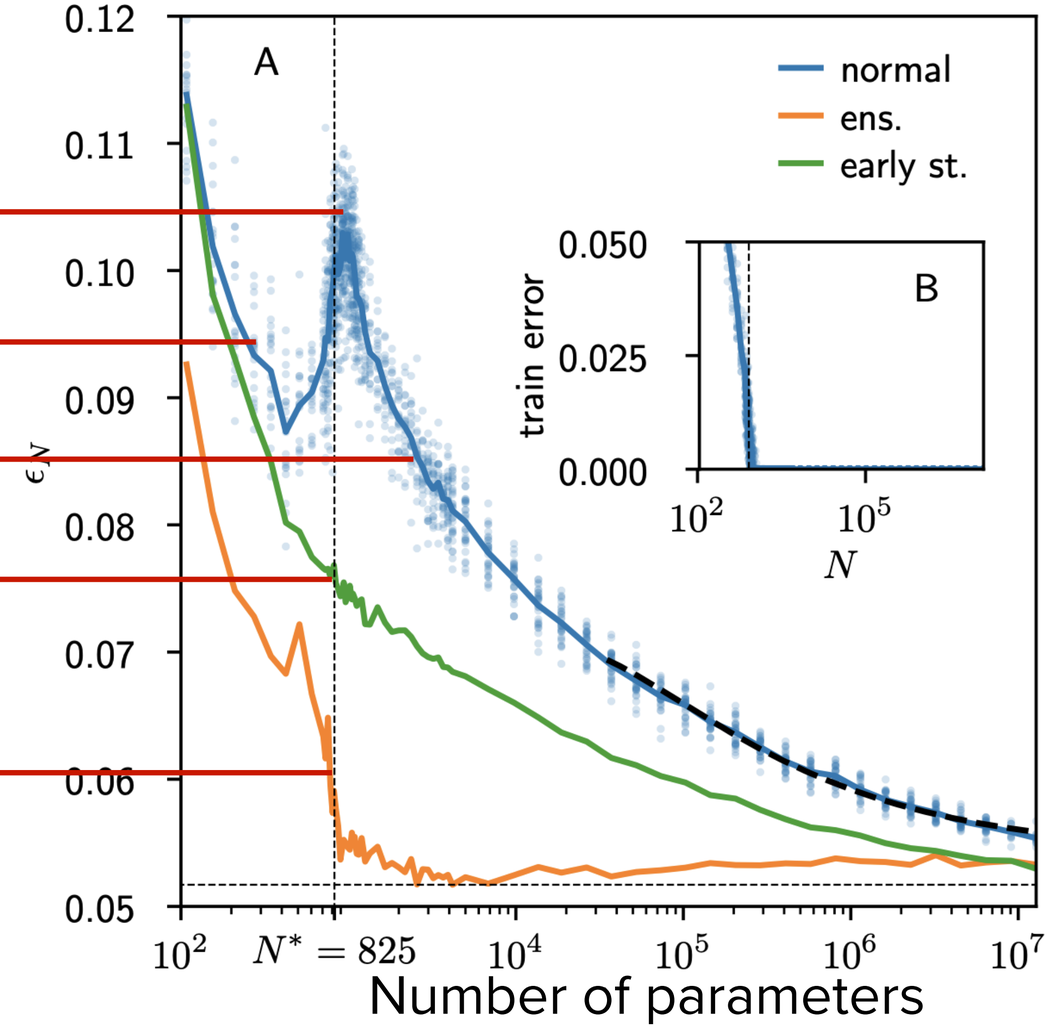
Peak suppressed by **ensembling**



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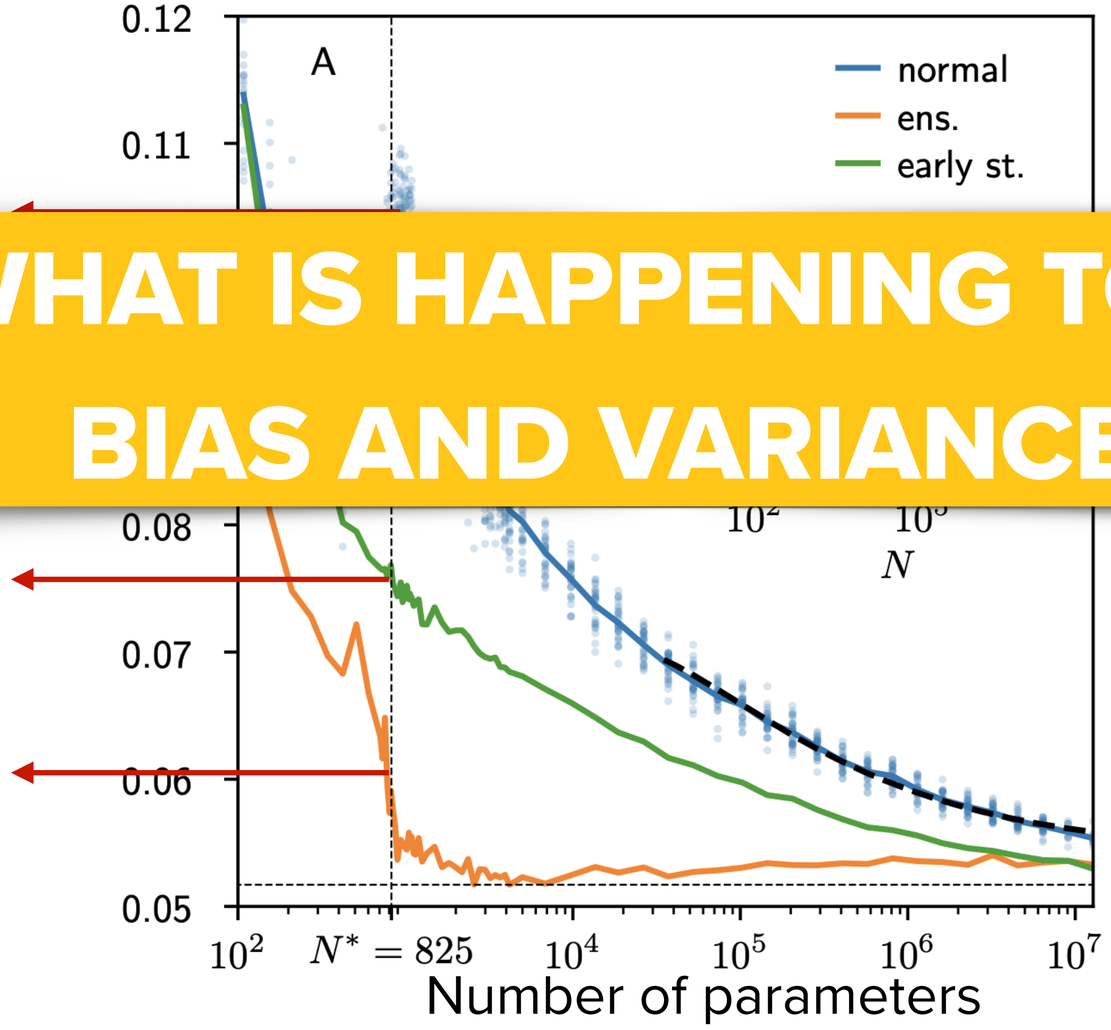

WHAT IS HAPPENING TO THE BIAS AND VARIANCES ?

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nari 2019

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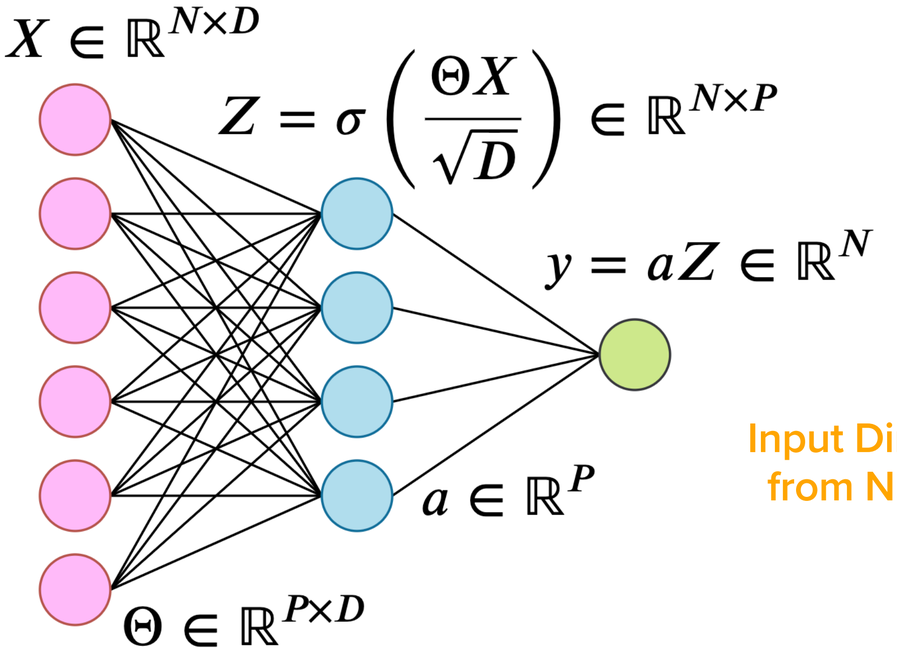
RANDOM FEATURES: WHY?



First introduced as **approximation** for **kernel methods [1]**

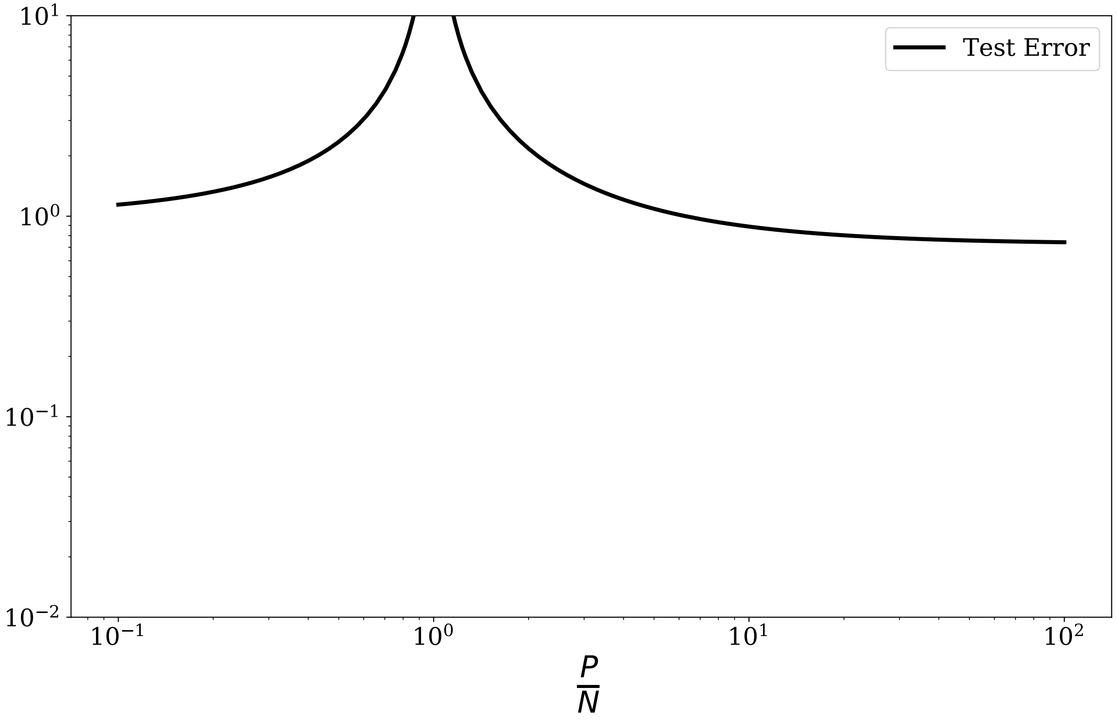
ANALYTICALLY TRACTABLE MODEL

- Input Dimension disentangled from Number of Parameters
- Double descent curve [2]
- Effect of Initialisation: Study Ensembling
- Relevant to the lazy regime of neural networks [3,4]

[1] Rahimi, Ali, and Benjamin Recht. "**Random features for large-scale kernel machines**." *Advances in neural information processing systems*. 2008.
[2] Mei, Song, and Andrea Montanari. "**The generalization error of random features regression: Precise asymptotics and double descent curve**." arXiv preprint arXiv:1908.05355 (2019).
[3] Arthur Jacot, Franck Gabriel, and Clément Hongler. **Neural tangent kernel: Convergence and generalization in neural networks**. In Advances in neural information processing systems, pages 8571–8580, 2018.
[4] Chizat, Lenaic, and Francis Bach. "**A note on lazy training in supervised differentiable programming**." arXiv preprint arXiv:1812.07956 8 (2018).

BIAS AND VARIANCE(S)

Analytical decomposition of the test error in random features regression



Analytical results for Random Feature Networks

BIAS AND VARIANCE(S)

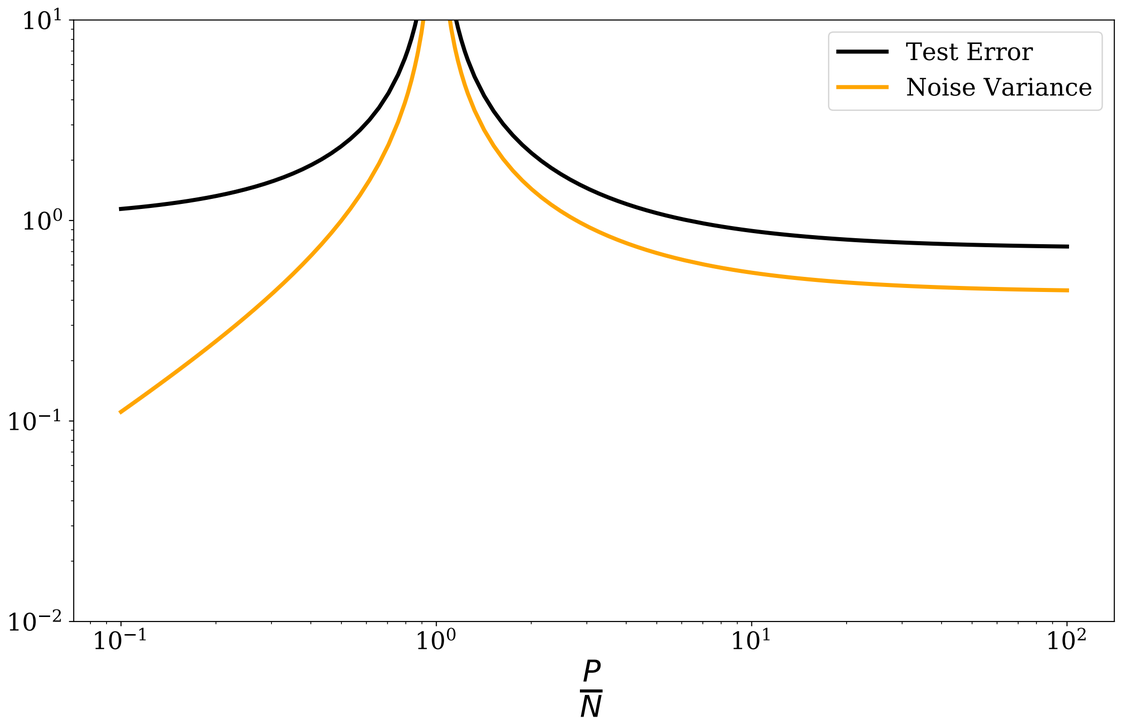
Analytical decomposition of the test error in random features regression

SOURCES OF RANDOMNESS

Label Noise

TEST ERROR

Noise Variance



Analytical results for Random Feature Networks

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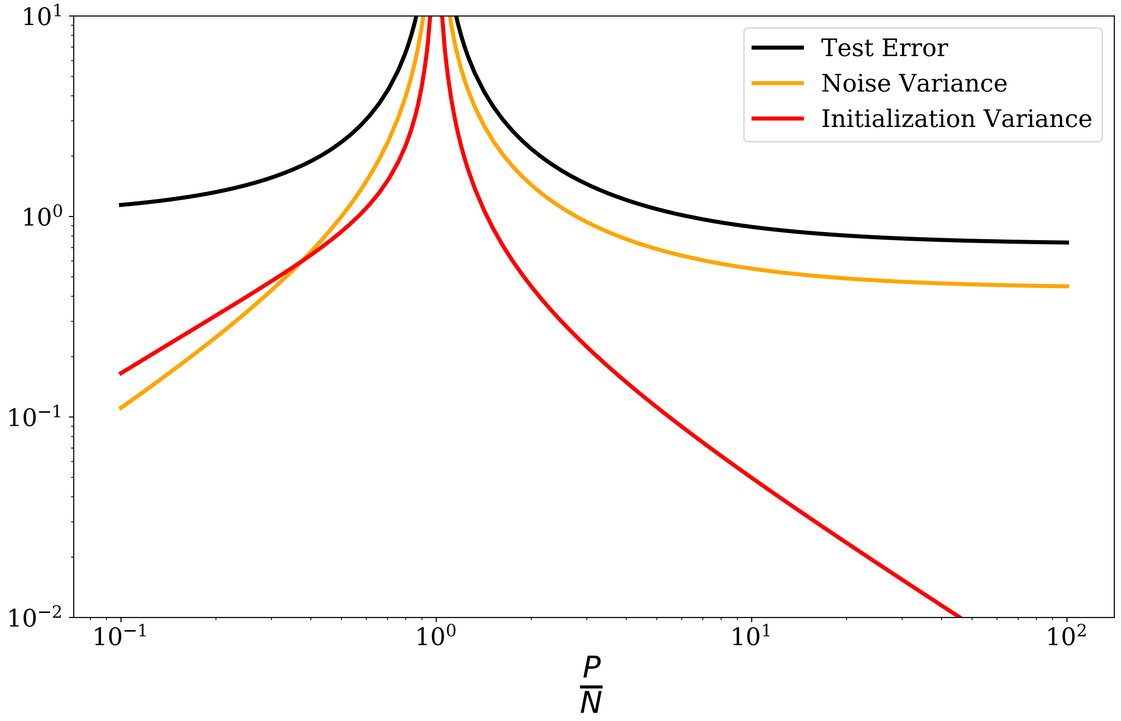
Features Initialisation

TEST ERROR

Noise Variance

Initialisation Variance



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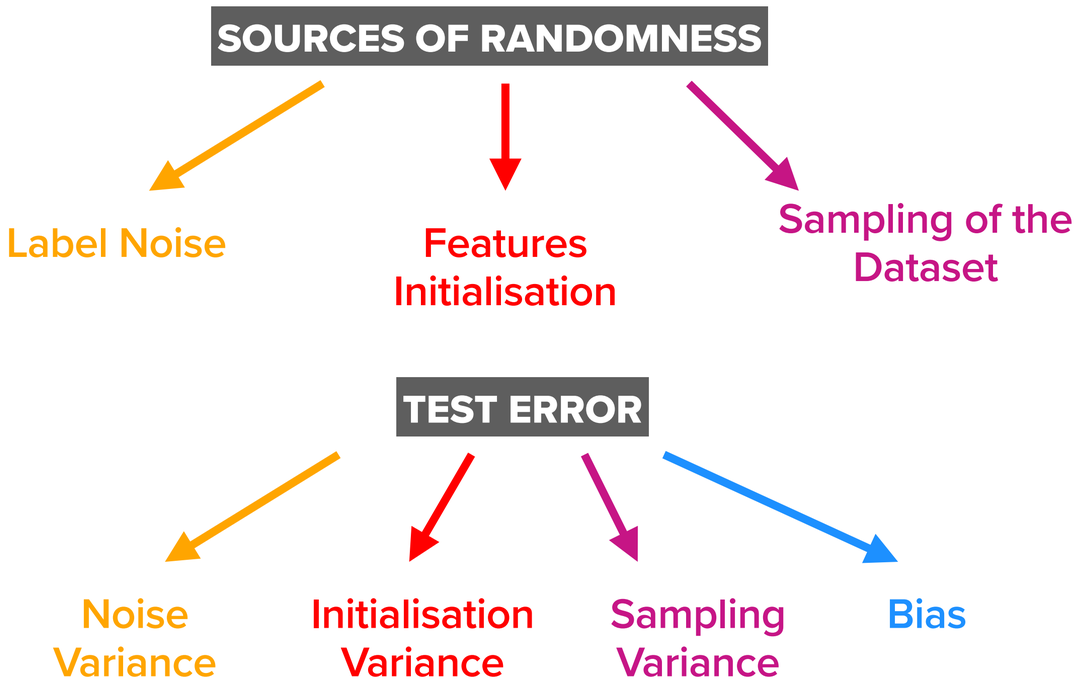

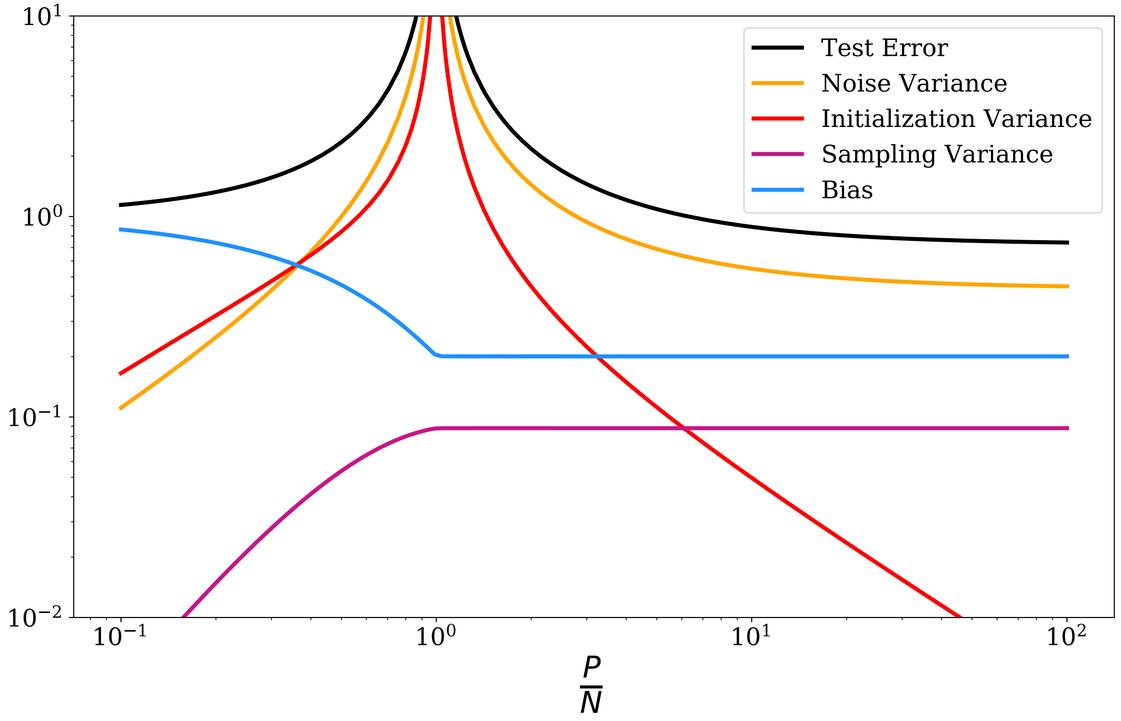

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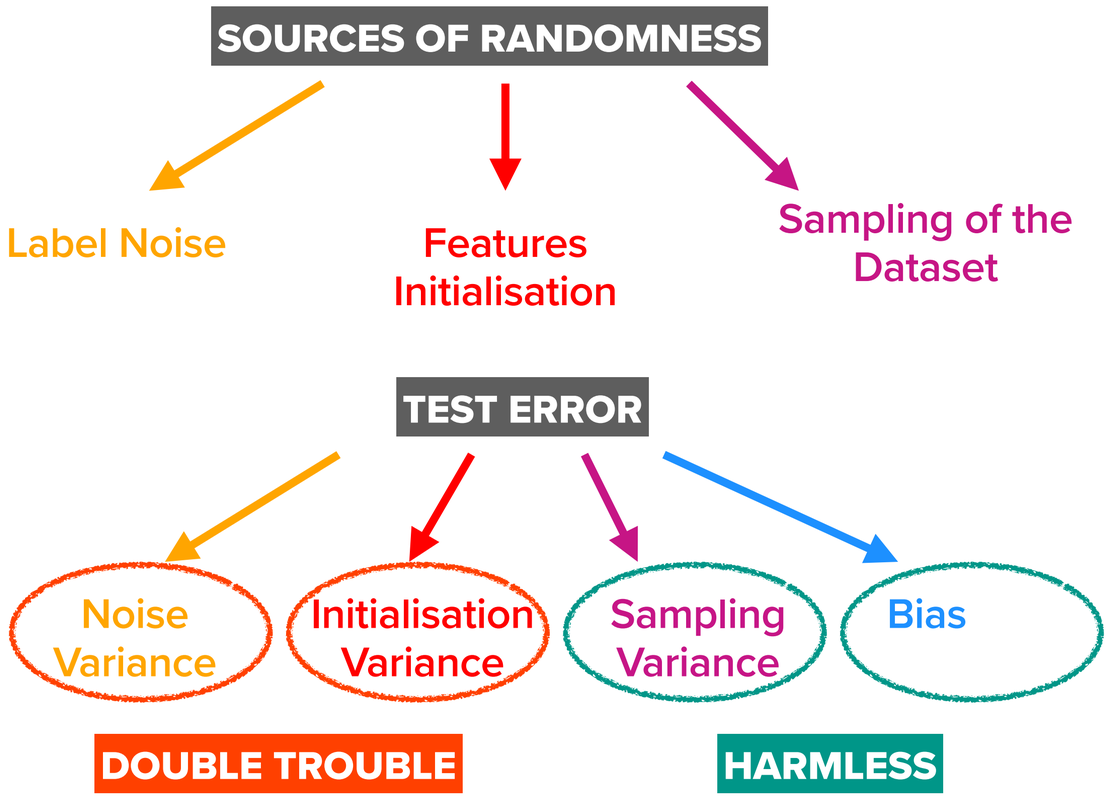
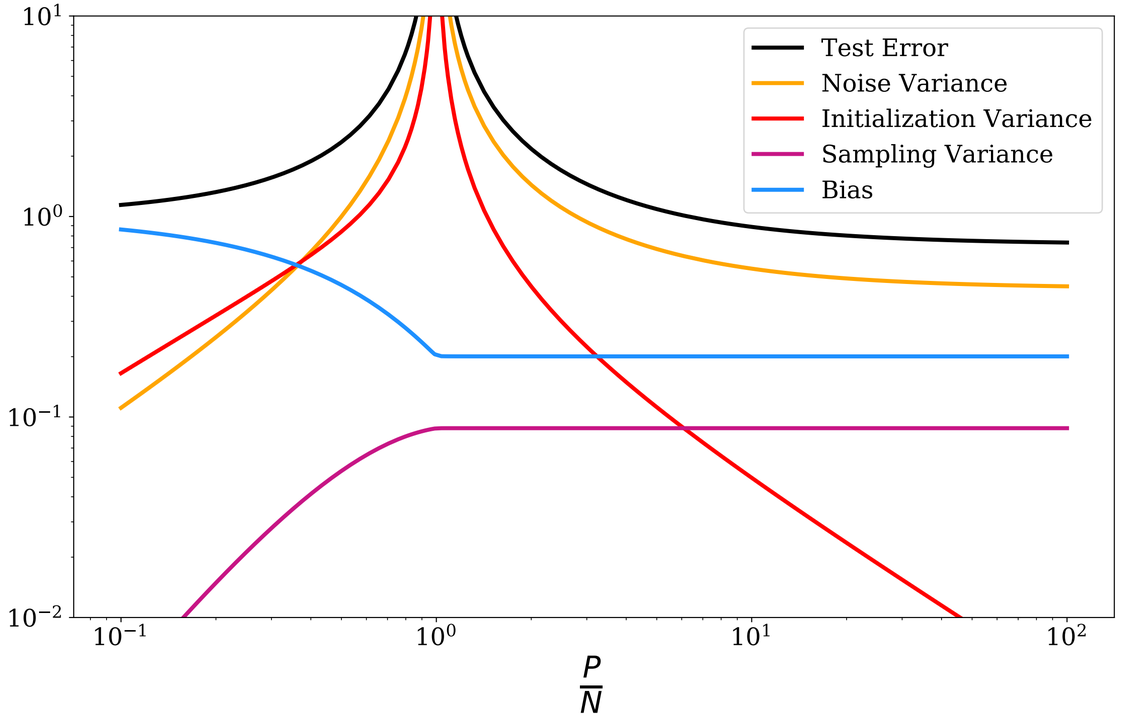
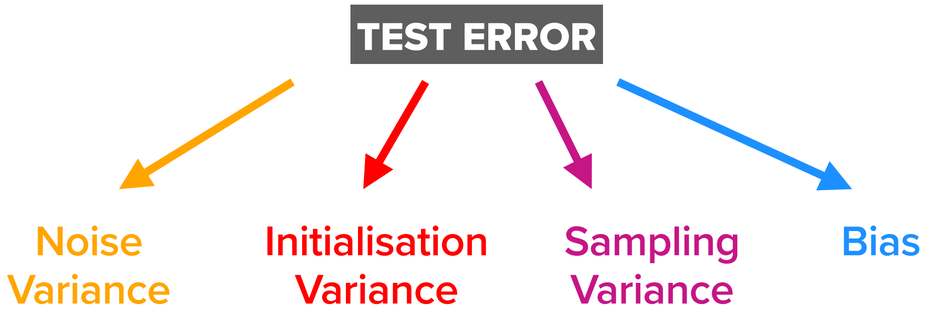
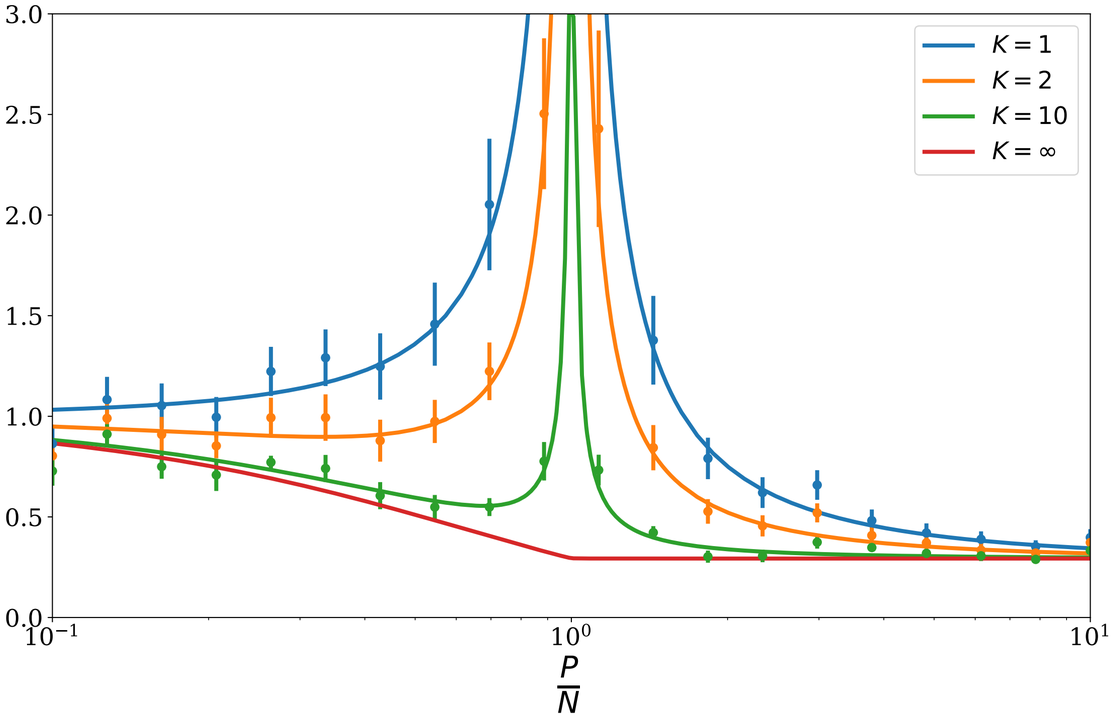




Analytical results for Random Feature Networks

ENSEMBLING





Analytical results for Random Feature Networks

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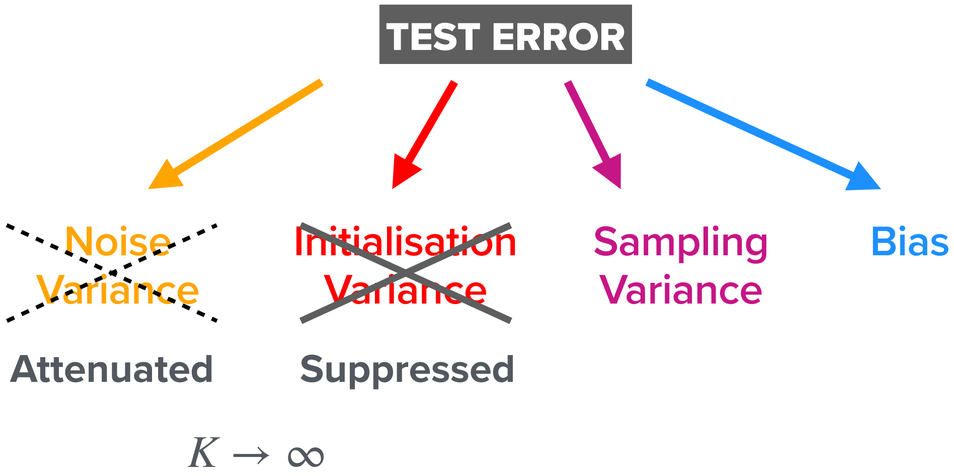
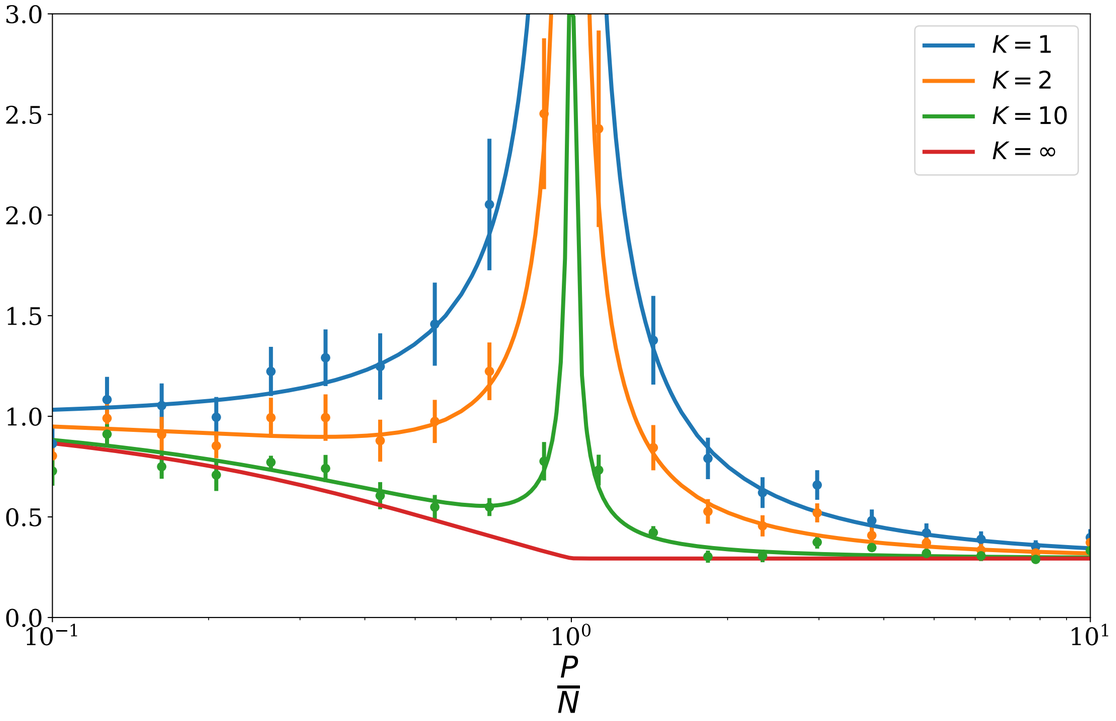
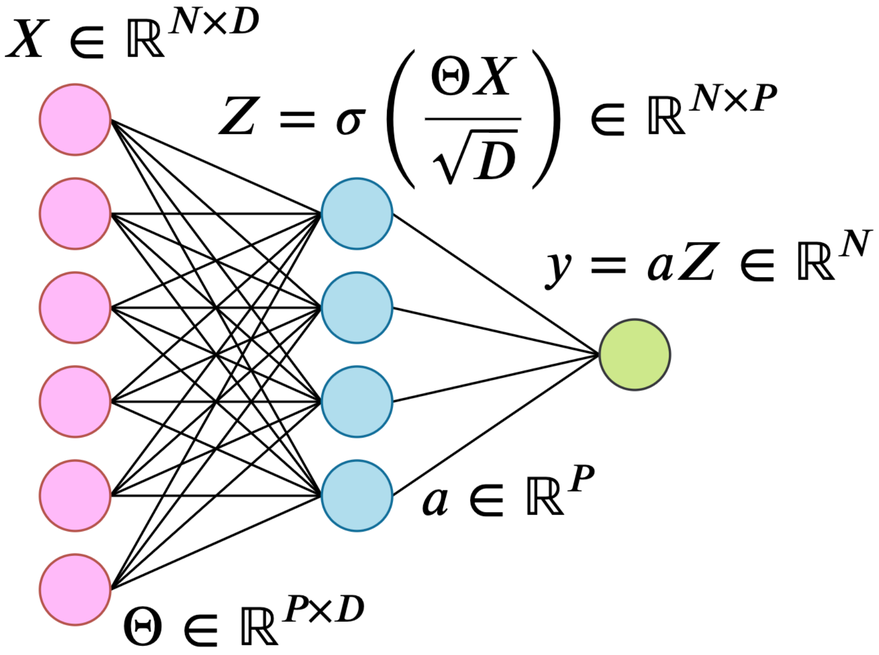




Analytical results for Random Feature Networks

THE RANDOM FEATURES MODEL



$\sigma = \text{ReLU}$ $\qquad$ $X, \boldsymbol{\Theta}, \boldsymbol{\beta} \sim \mathcal{N}(0,1)$

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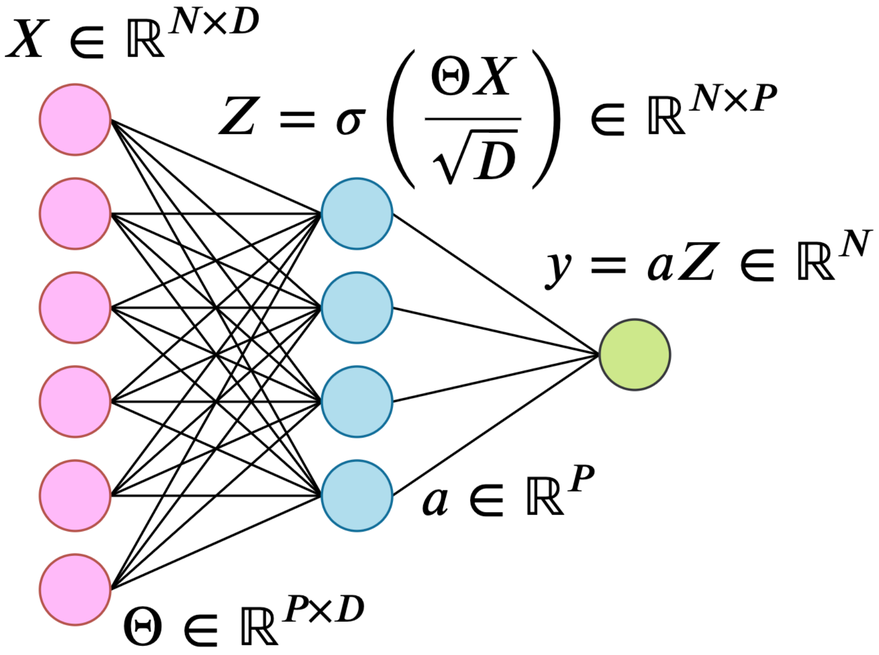

LEARNER: ONE HIDDEN LAYER

$$\hat{f}(X_\mu) = \sum_{i=1}^{P} a_i \sigma\left(\frac{\langle \Theta_i, X_\mu \rangle}{\sqrt{D}}\right)$$

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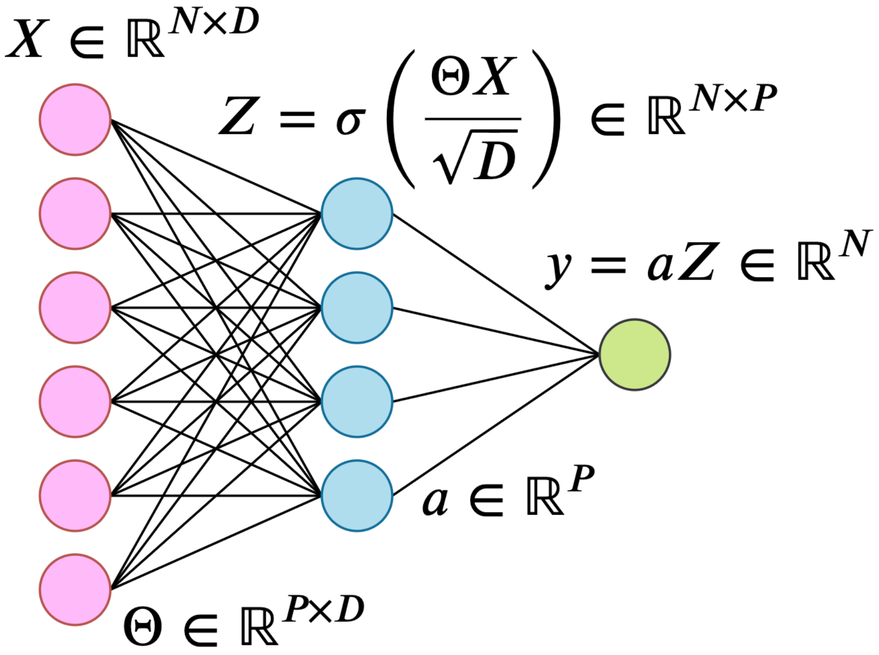

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GROUND TRUTH: LINEAR WITH NOISE

$$y_\mu = f(X_\mu) = \langle \boldsymbol{\beta}, X_\mu \rangle + \epsilon_\mu$$

$$\|\boldsymbol{\beta}\| = F, \quad \epsilon_\mu \sim \mathcal{N}(0,\tau)$$

$$\mathrm{SNR} = F/\tau$$

$\sigma = \mathrm{ReLU}$ $\qquad$ $X, \Theta, \boldsymbol{\beta} \sim \mathcal{N}(0,1)$

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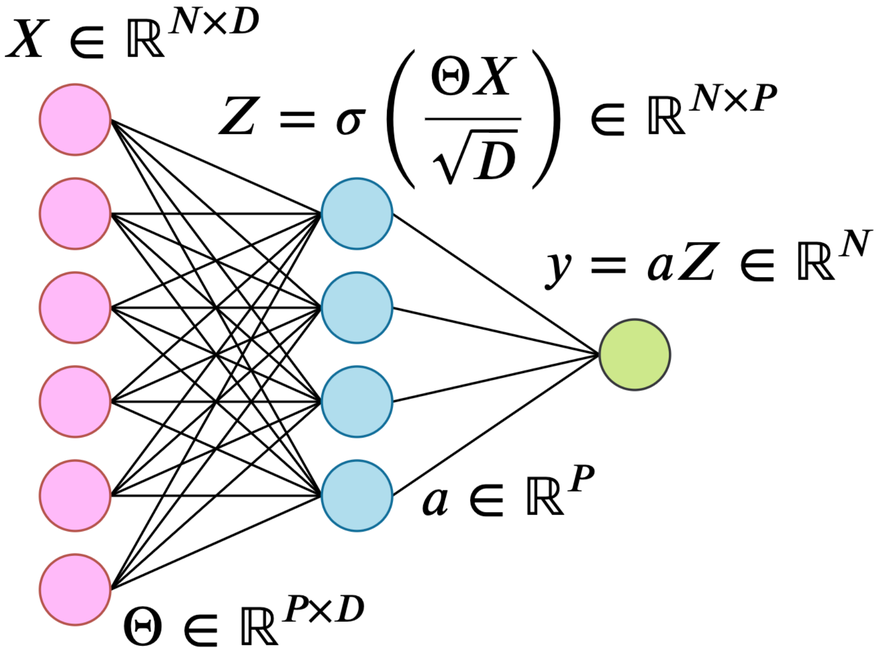

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TRAIN ERROR

$$\mathscr{L}_{\mathrm{RF}}(\boldsymbol{a}) \equiv \frac{1}{N}\sum_{\mu=1}^{N}\left(y_\mu - \hat{f}(\boldsymbol{X}_\mu)\right)^2 + \frac{P\lambda}{D}\|\boldsymbol{a}\|_2^2$$

$$\hat{\boldsymbol{a}} \equiv \arg\min_{\boldsymbol{a}\in\mathbb{R}^P} \mathscr{L}_{\mathrm{RF}}(\boldsymbol{a})$$

$\sigma = \mathrm{ReLU}$ $\qquad$ $\boldsymbol{X}, \boldsymbol{\Theta}, \boldsymbol{\beta} \sim \mathcal{N}(0,1)$

THE RANDOM FEATURES MODEL

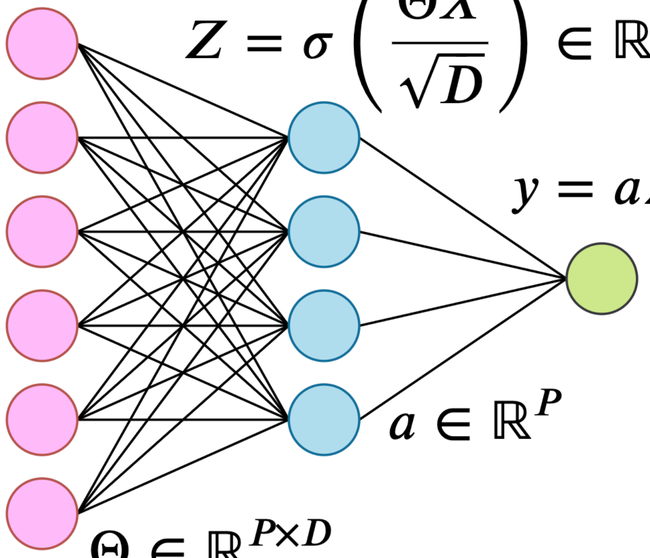
$X \in \mathbb{R}^{N \times D}$

$Z = \sigma\left(\frac{\Theta X}{\sqrt{D}}\right) \in \mathbb{R}^{N \times P}$

$y = aZ \in \mathbb{R}^{N}$

$a \in \mathbb{R}^{P}$

$\Theta \in \mathbb{R}^{P \times D}$



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$$\hat{a} \equiv \arg\min_{a \in \mathbb{R}^P} \mathcal{L}_{\mathrm{RF}}(a)$$

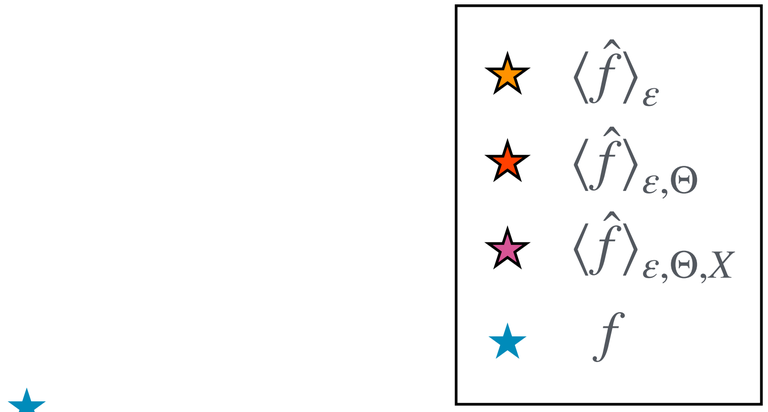
TEST ERROR

$$\mathcal{R}_{\mathrm{RF}} = \mathbb{E}_x \left[\left(f(x) - \hat{f}(x)\right)^2\right]$$

BIAS AND VARIANCE(S)

$$\mathscr{R}_{\mathrm{RF}} = \mathbb{E}\left[\left(f - \hat{f}\right)^2\right]$$

$$= F^2 + 2\mathbb{E}\left[f\hat{f}\right] + \mathbb{E}\left[\hat{f}^2\right]$$



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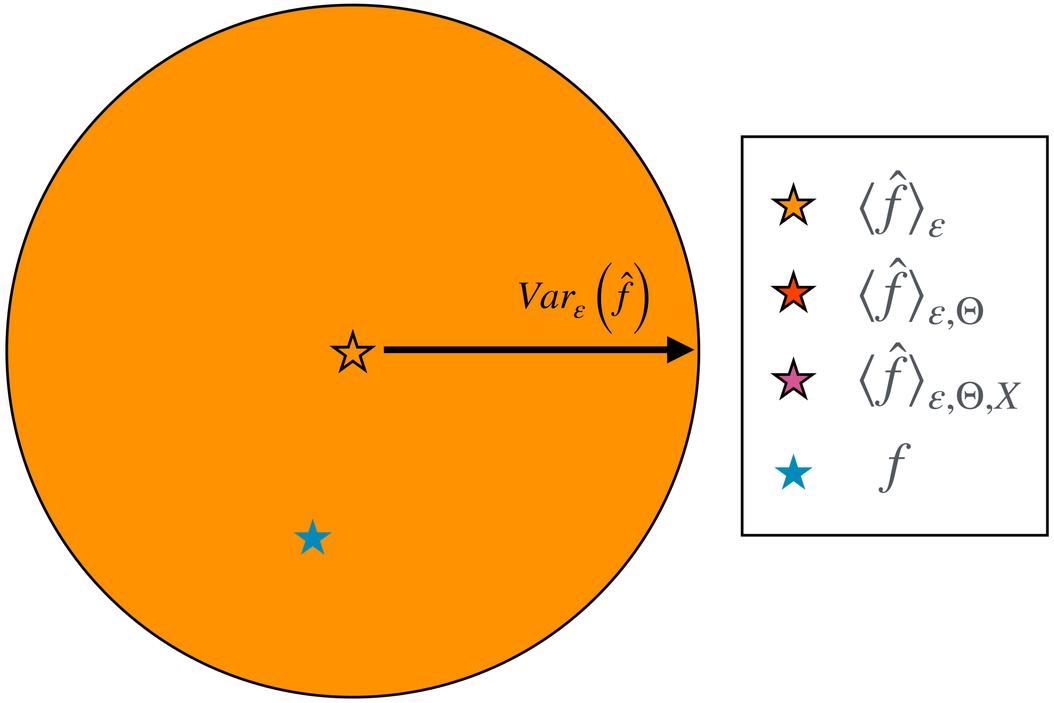

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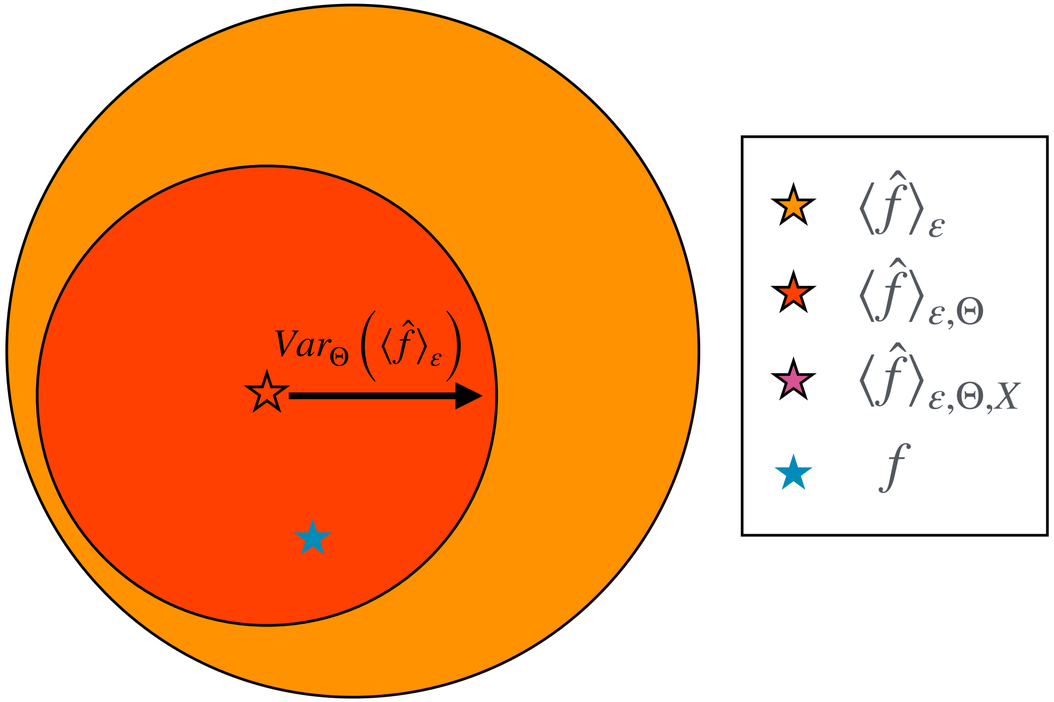

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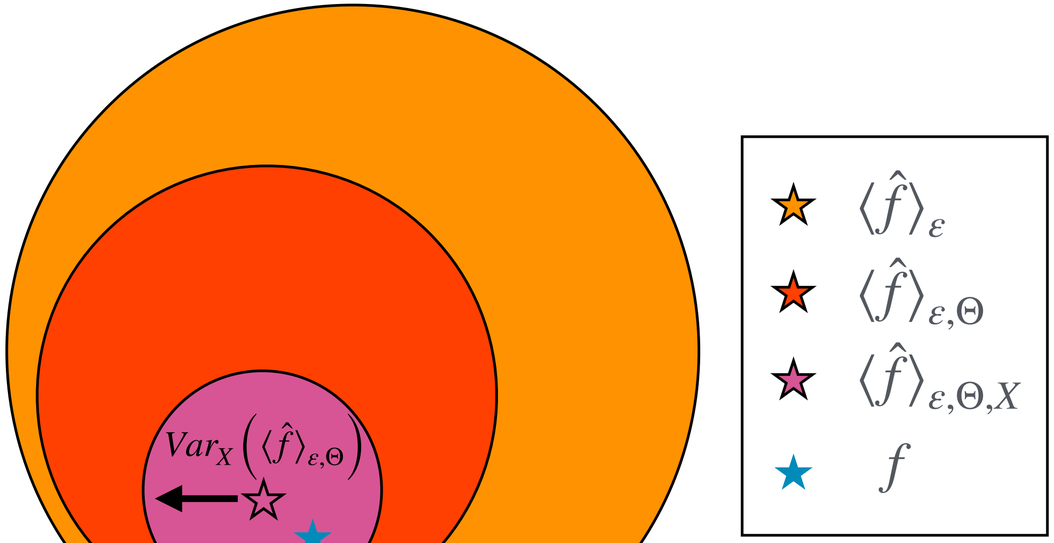
Noise **Initialization** **Sampling**



ANALYTIC THEORY

We provide an asymptotic formula in the high-dimensional limit $N, P, D \to \infty, \quad \frac{P}{D} = \mathcal{O}(1), \quad \frac{N}{D} = \mathcal{O}(1)$

- **Vanilla** terms
  mean & fluct of vanilla learner:
  both **diverge** at the interpolation threshold

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  mean & fluct of init+samp-averaged learner:
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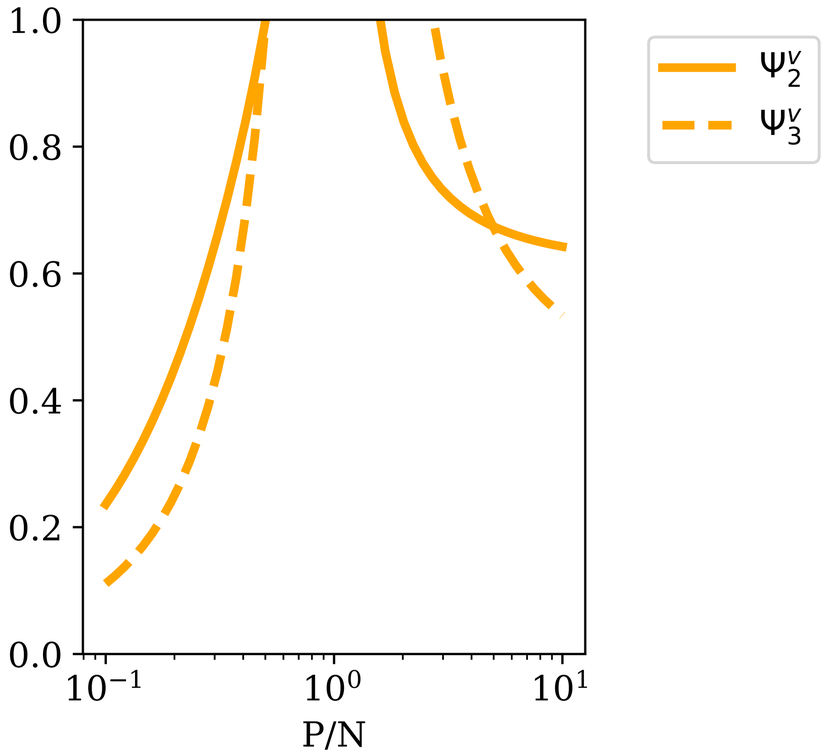

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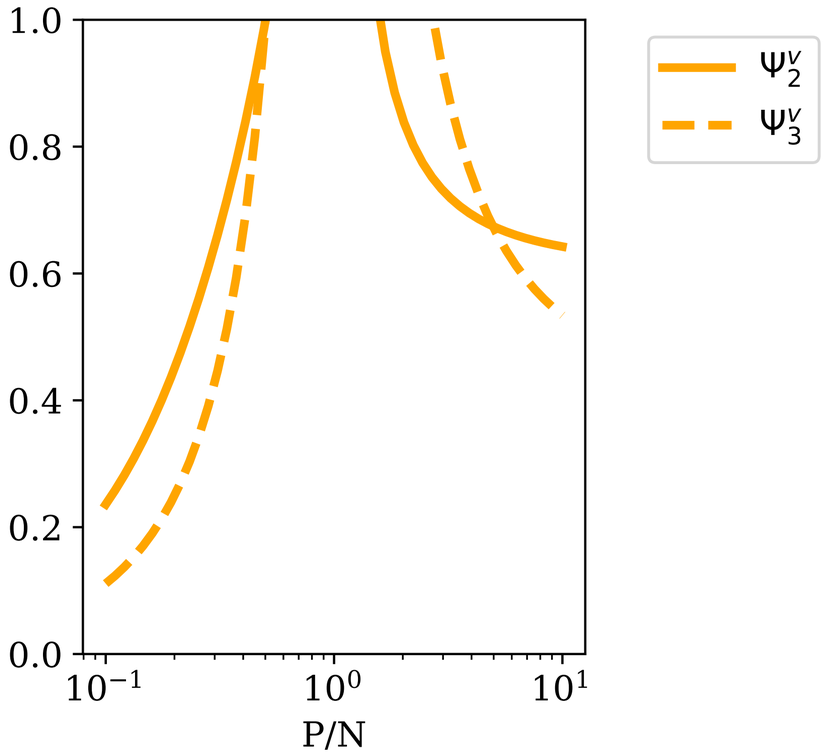

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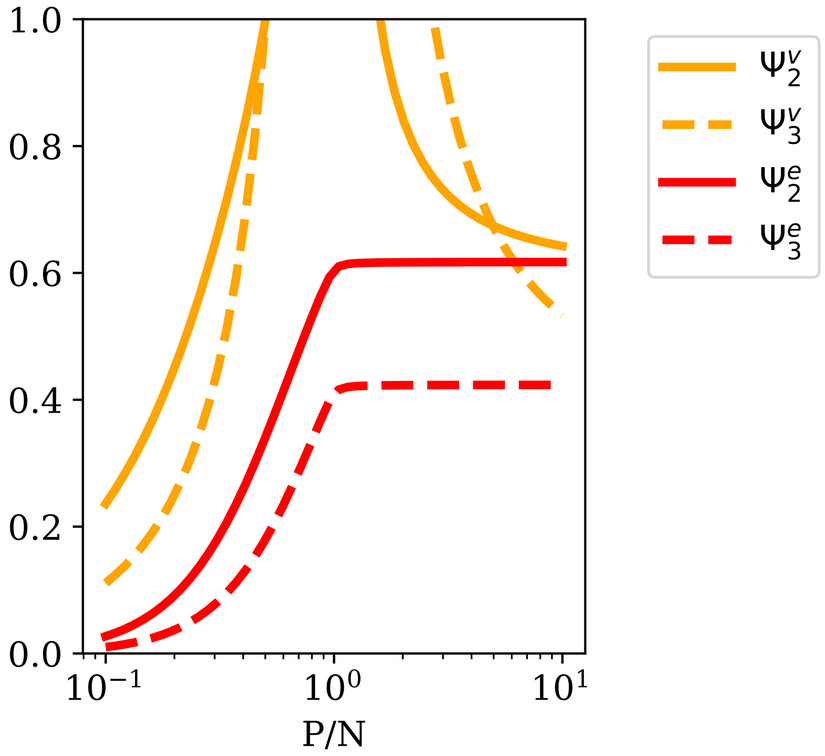

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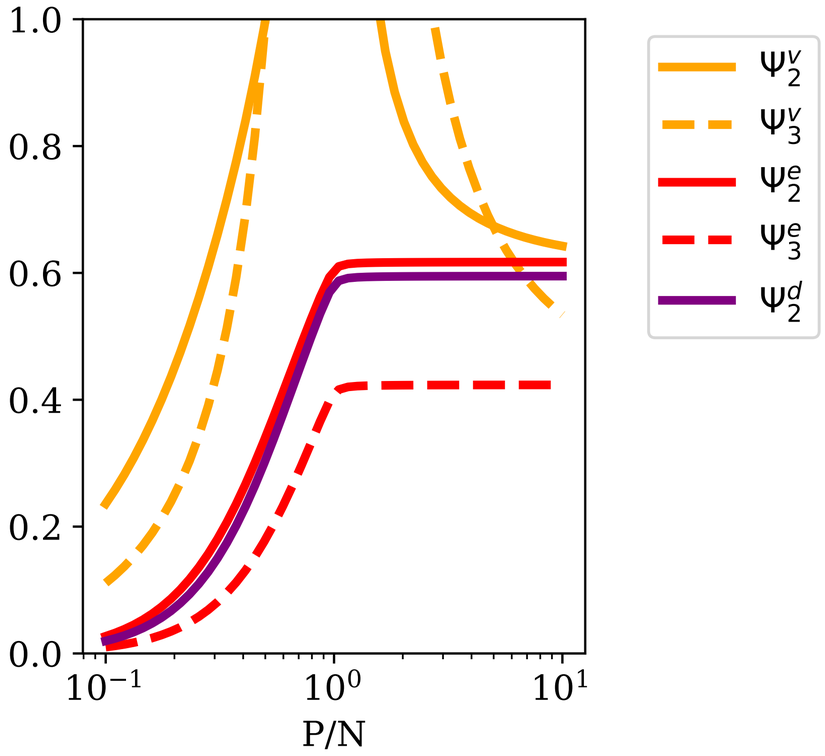
NEW



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BIAS AND VARIANCES

Decomposition of the test error $\mathop{\mathbb{E}}_{\boldsymbol{\Theta},X,\boldsymbol{\varepsilon}}\left[\mathscr{R}_{\mathrm{RF}}\right] = Var_{\mathrm{Noise}} + Var_{\mathrm{Init}} + Var_{\mathrm{Samp}} + Bias$

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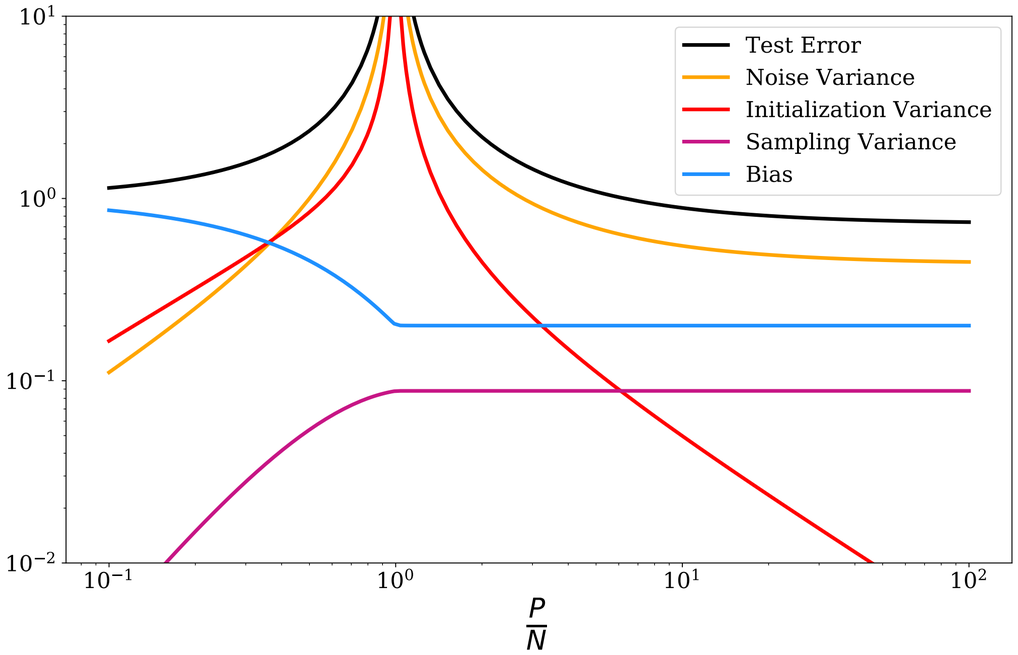

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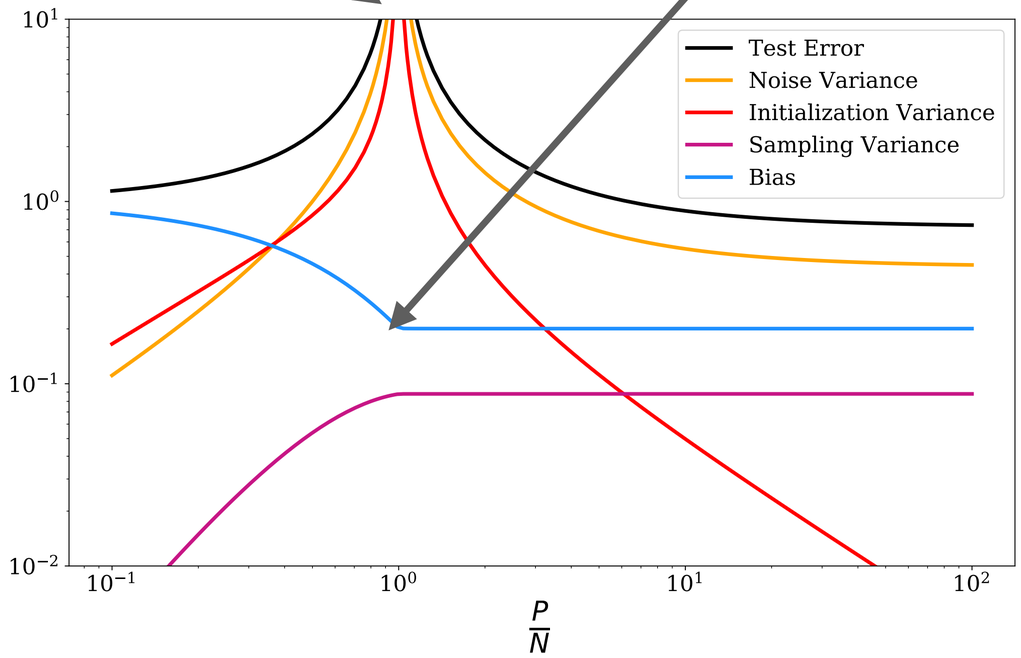

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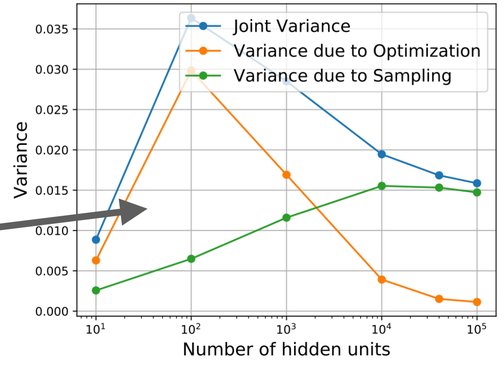
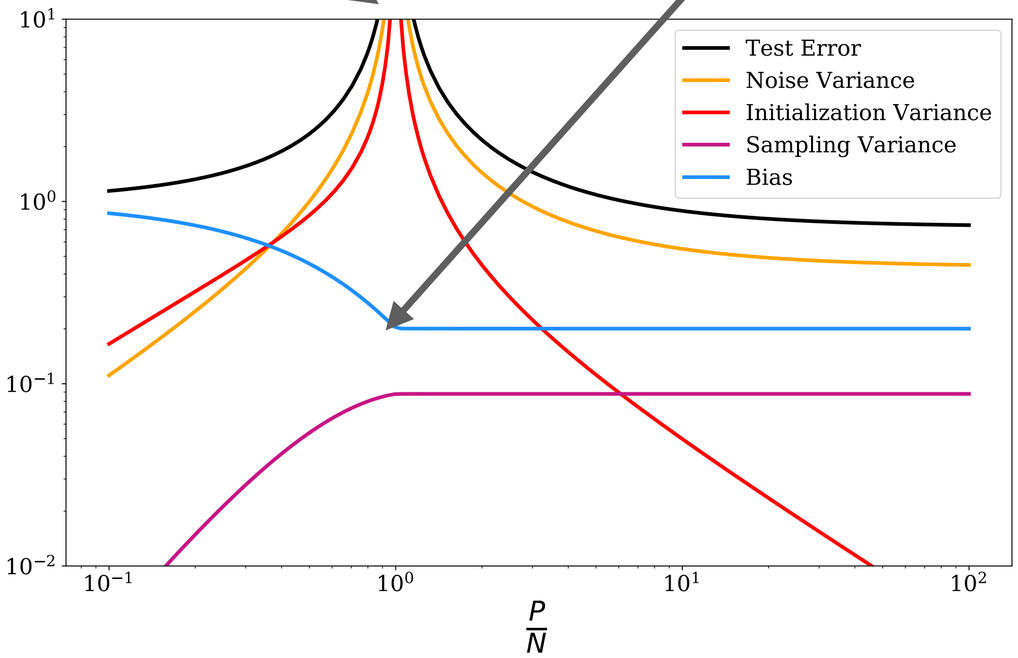
CONSISTENT WITH EMPIRICAL STUDY IN NEURAL NETWORKS [2]

Init variance peaks,
Sampling variance plateaus





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EFFECT OF ENSEMBLING

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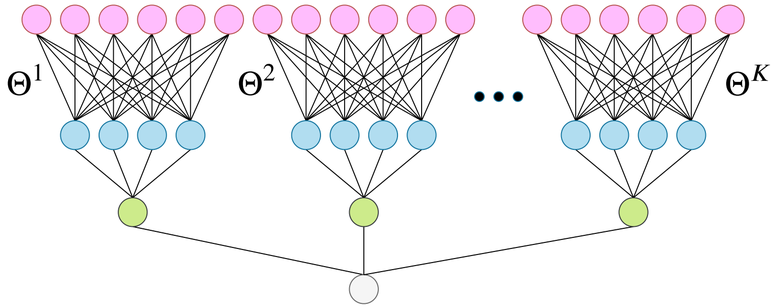

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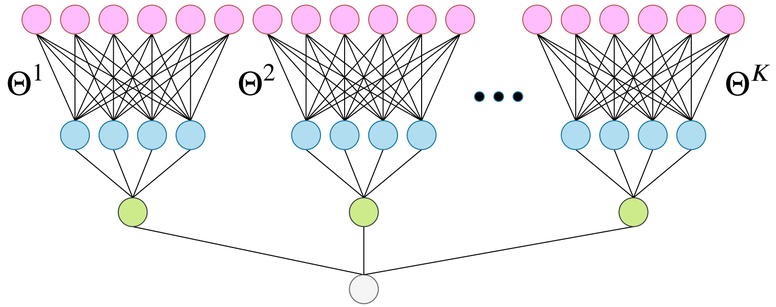

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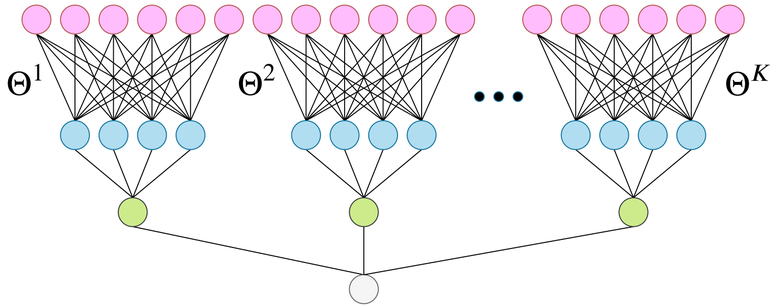
VANILLA TERMS SUPPRESSED AS $1/K$



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LINEAR INTERPOLATION TO ENSEMBLING TERMS

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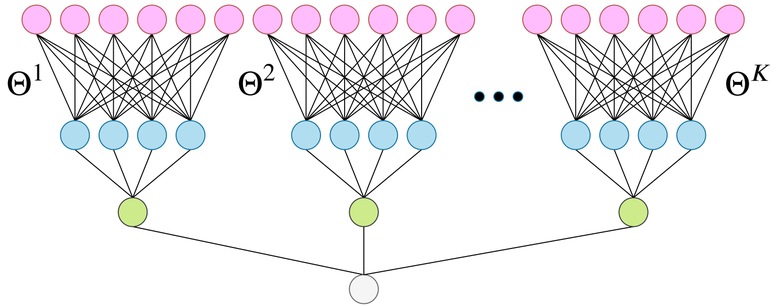

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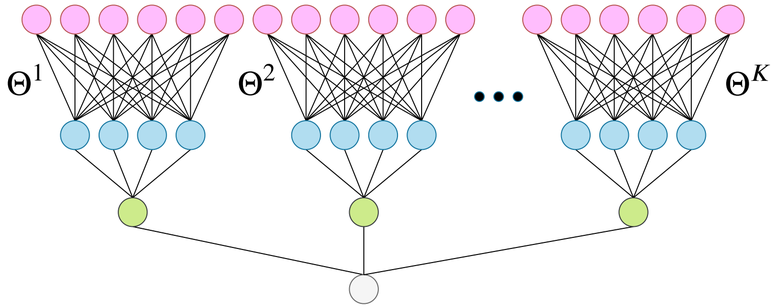
CONSISTENT WITH EMPIRICAL STUDY IN NEURAL NETWORKS [1]



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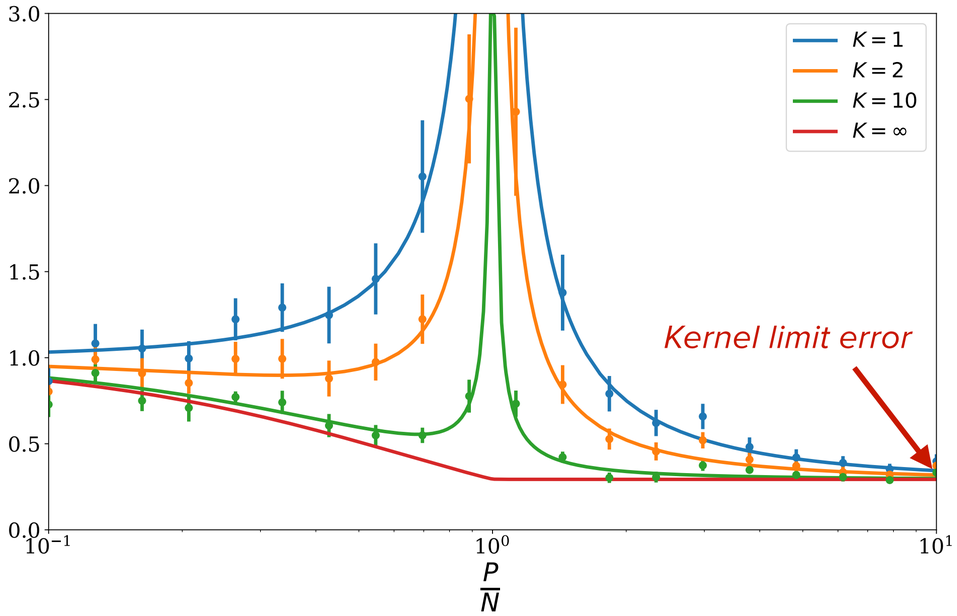

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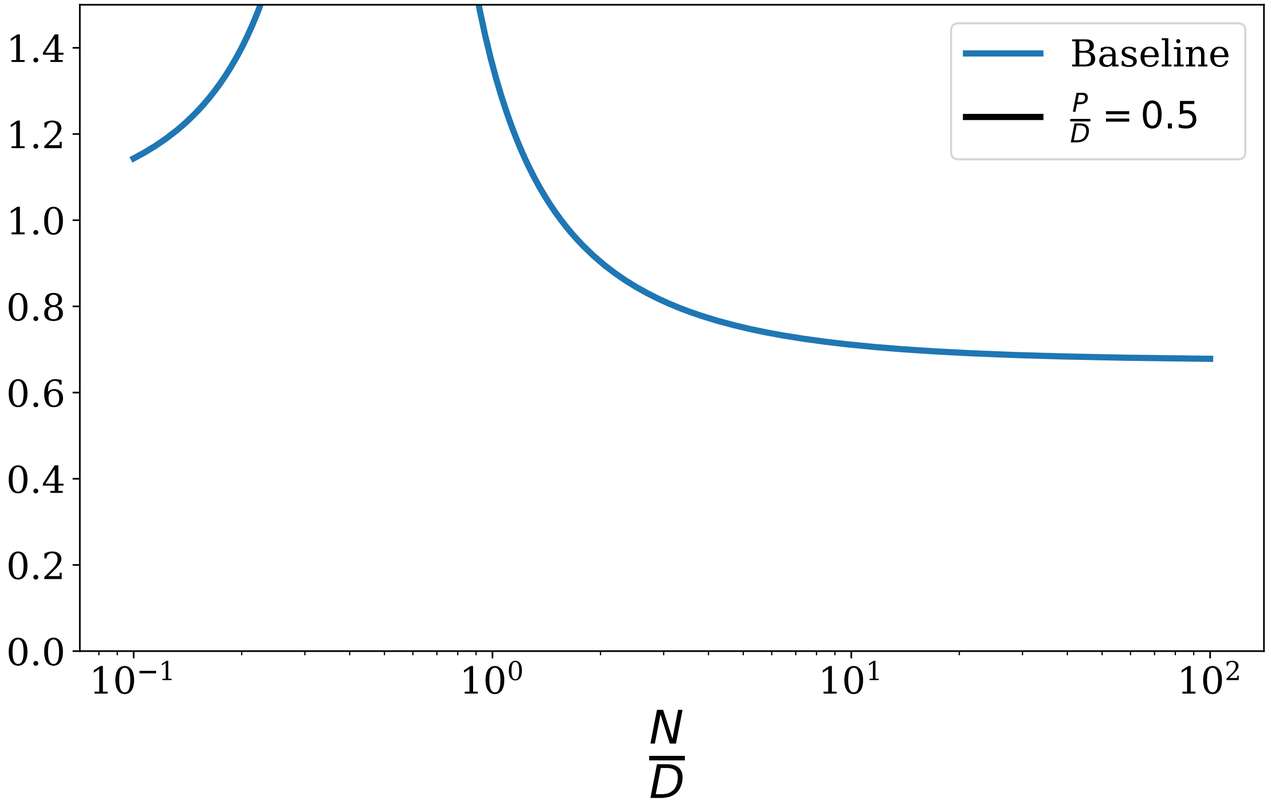
Which is better: doubling the number of features or ensembling 2 networks ?



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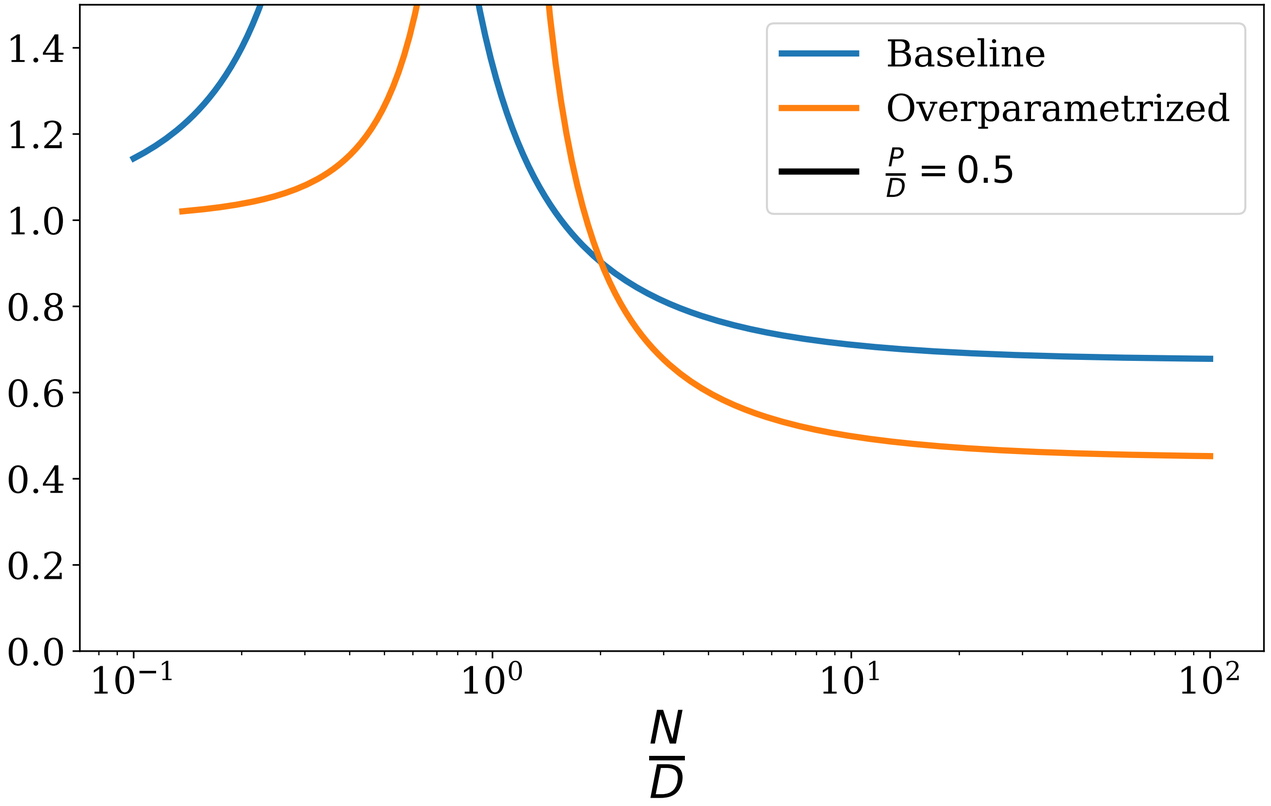

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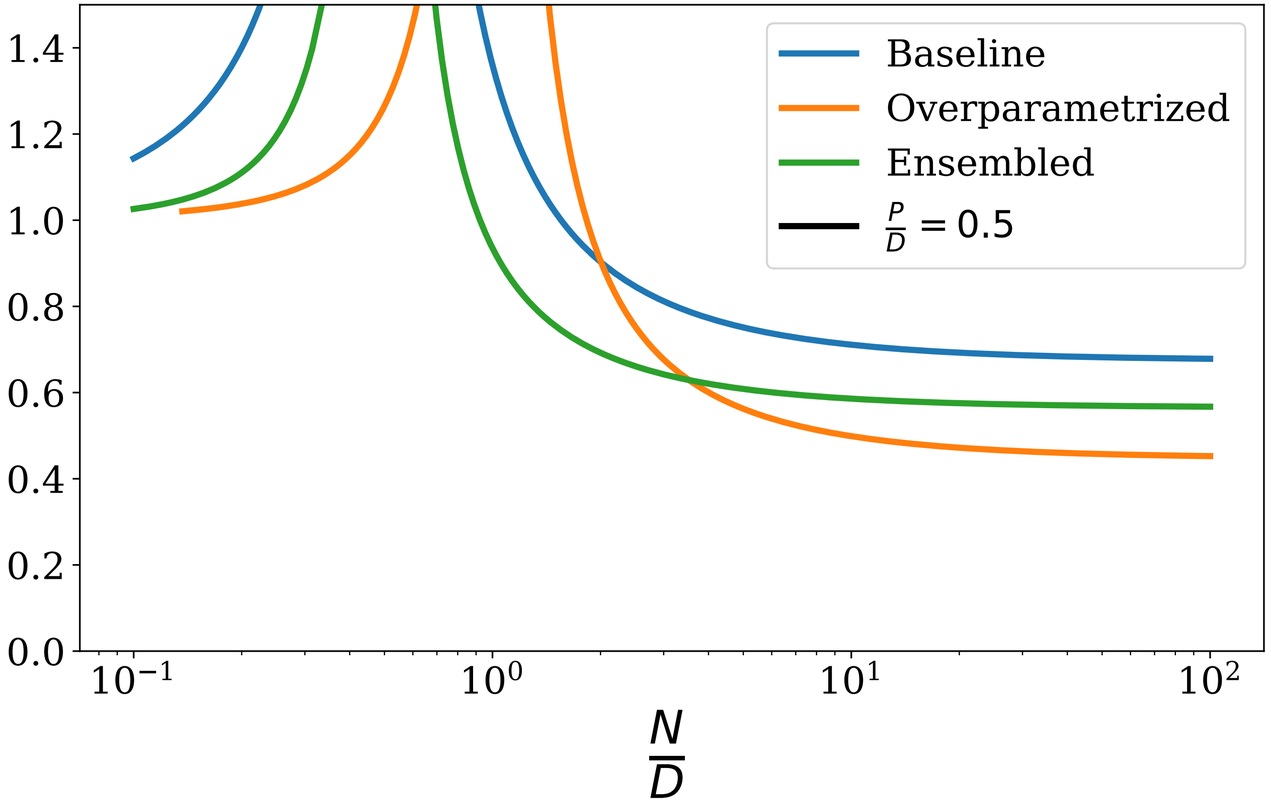

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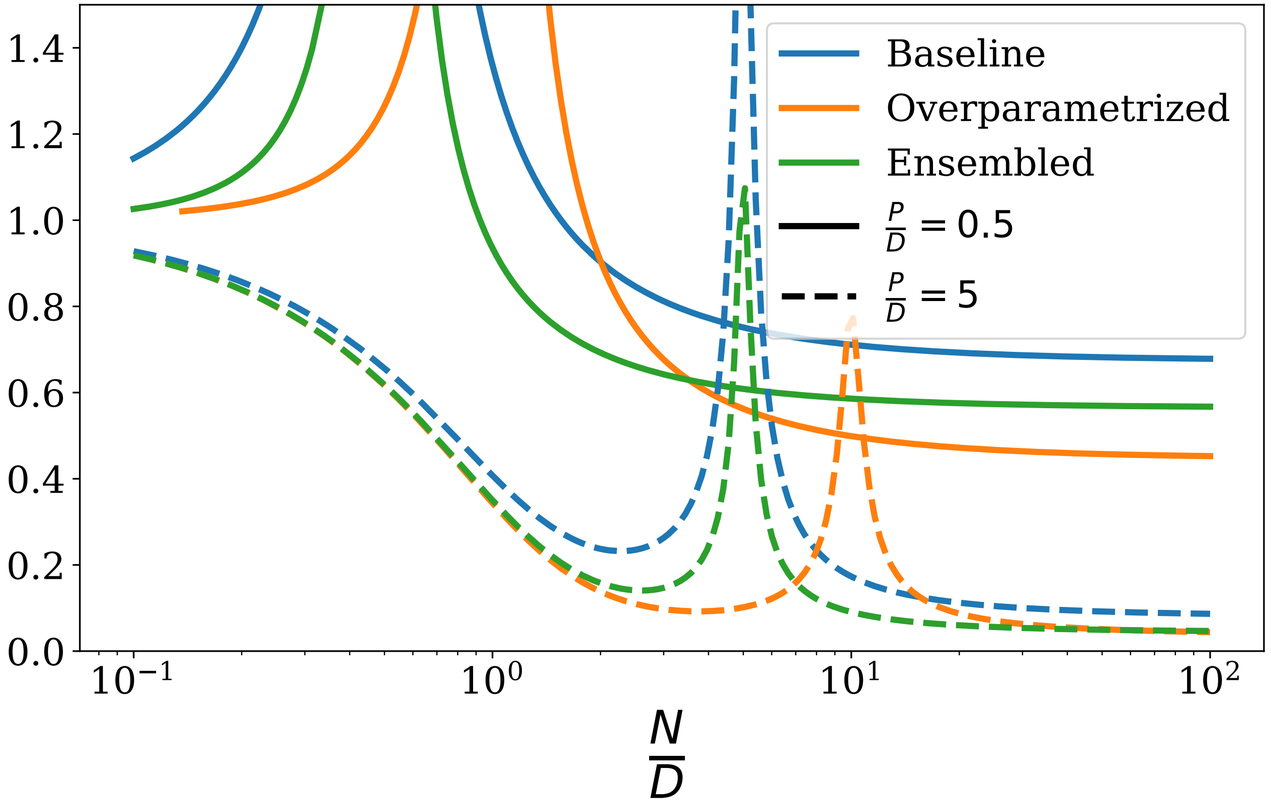

Overparametrizing is better (but slower!)

Except when already overparametrized

ENSEMBLING VS DIVIDE AND CONQUER

Ensembling:

Train K learners on same dataset

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Each learner has less data BUT noise term disappears as $K \to \infty$

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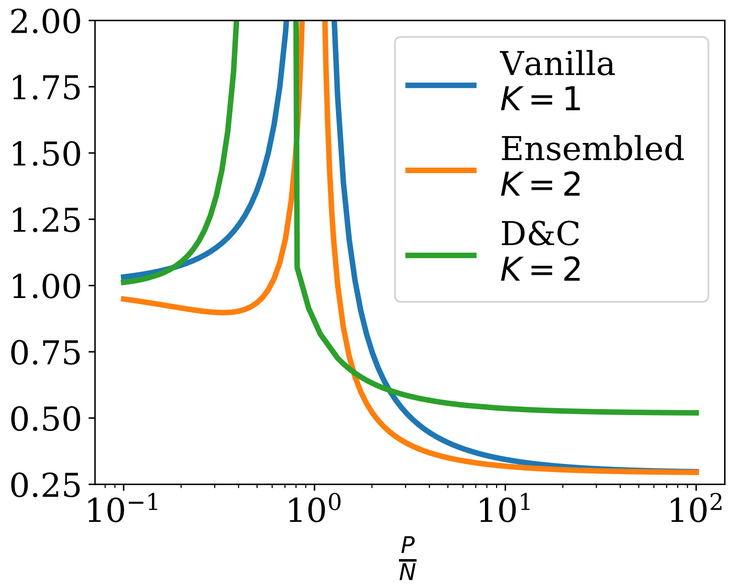
Ensembling:

Train K learners on same dataset

$$\mathop{\mathbb{E}}_{\Theta,X,\varepsilon}\left[\mathscr{R}_{\mathrm{RF}}\right] = F^2\left(1-2\Psi_1^v\right) + \frac{1}{K}\left(F^2\Psi_2^v + \tau^2\Psi_3^v\right) + \left(1-\frac{1}{K}\right)\left(F^2\Psi_2^e + \tau^2\Psi_3^e\right)$$

BETTER AT LOW NOISE



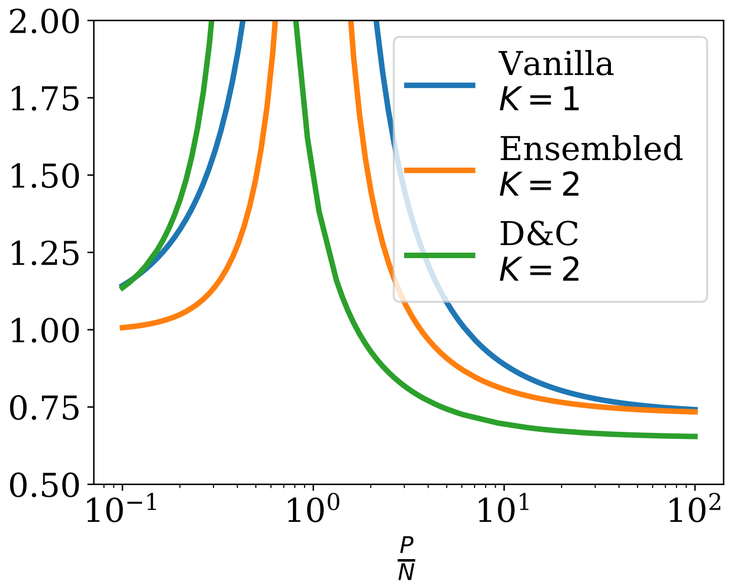
Divide and conquer:

Train on different splits of the dataset

$$\mathop{\mathbb{E}}_{\Theta,X,\varepsilon}\left[\mathscr{R}_{\mathrm{RF}}\right] = F^2\left(1-2\Psi_1^v\right) + \frac{1}{K}\left(F^2\Psi_2^v + \tau^2\Psi_3^v\right) + \left(1-\frac{1}{K}\right)F^2\Psi_2^d$$

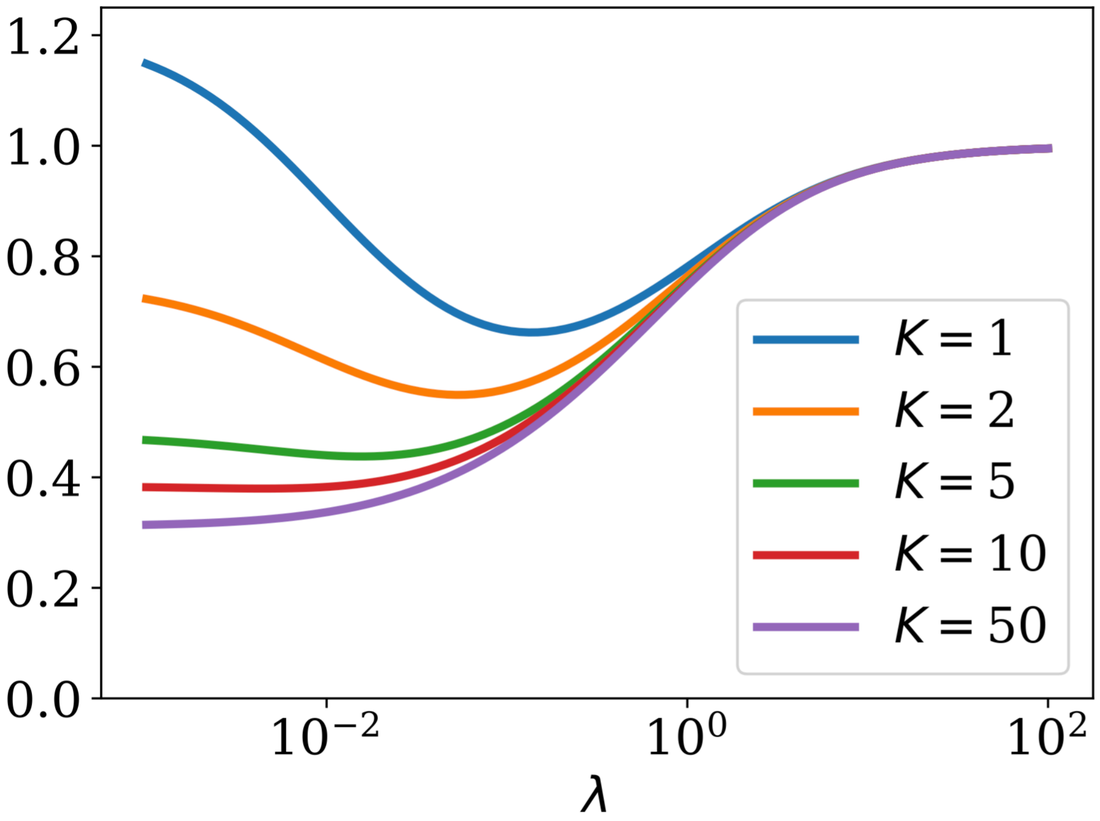
Each learner has less data BUT noise term disappears as $K \to \infty$

BETTER AT HIGH NOISE

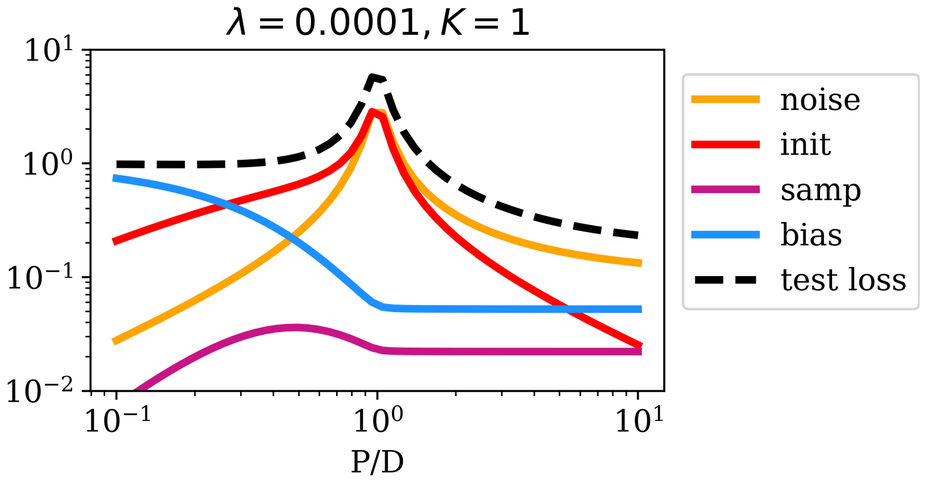


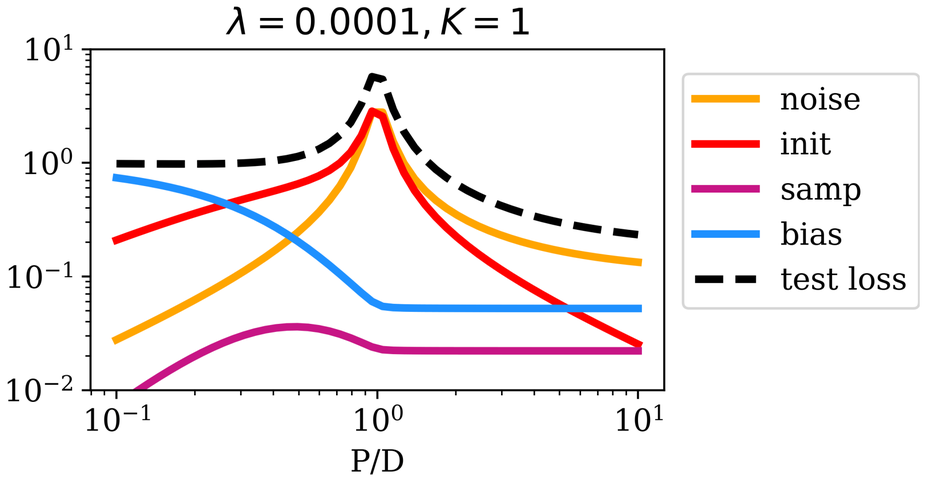
ENSEMBLING VS REGULARIZING

Ensembled learners are better off **under-regularised**



Ensembling also **reduces the variance**, but it also **increases the bias**





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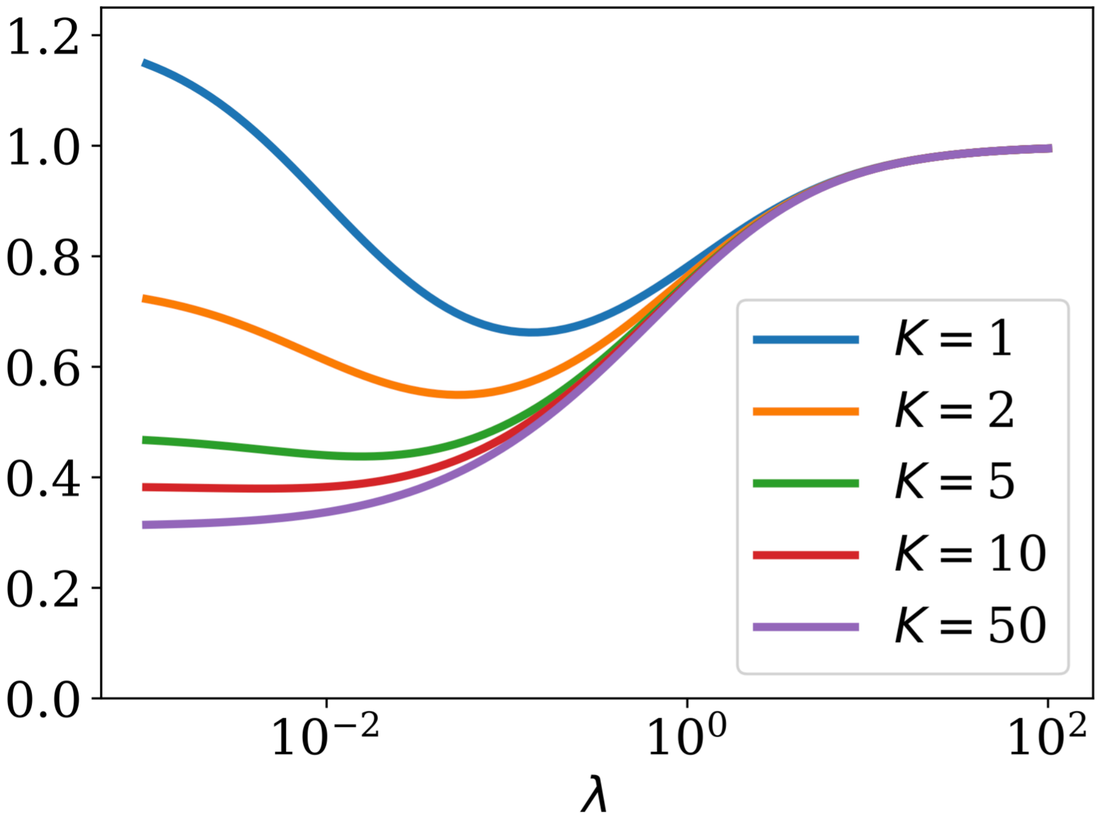

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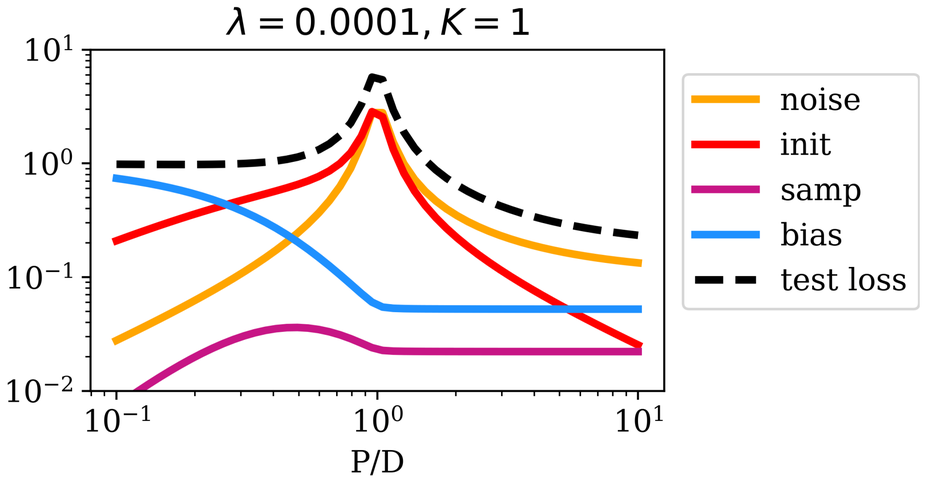
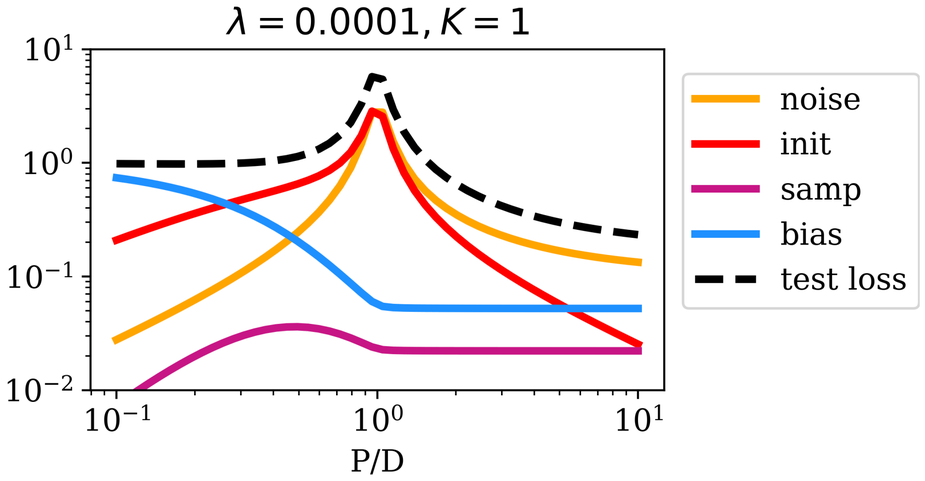




LAZY REGIME OF NEURAL NETWORKS

The lazy regime of neural network (weights move little) is equivalent to random feature regression:

$$f_\theta(\boldsymbol{x}) \approx \underbrace{f_{\theta_0}(\boldsymbol{x})}_{\text{Assume to be = 0}} + \underbrace{\nabla_\theta f_\theta(\boldsymbol{x})\Big|_{\theta=\theta_0}}_{\text{Random features}} \cdot \underbrace{(\theta - \theta_0)}_{\text{Vector to be learnt}}$$

We can enforce lazy behaviour by scaling the output of the network:

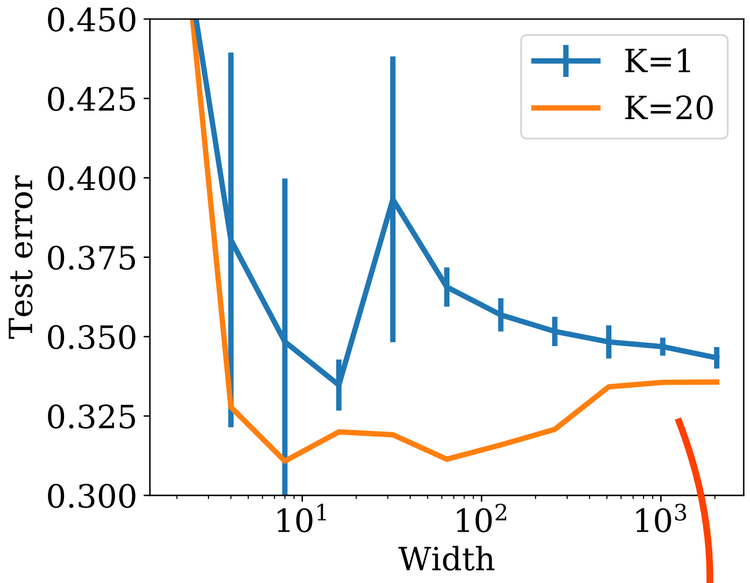
$$\underbrace{\alpha(f_\theta(\boldsymbol{x}) - f_{\theta_0}(\boldsymbol{x}))}_{\text{Must be of order one}} \approx \alpha \nabla f_{\theta_0}(\boldsymbol{x}) \cdot \underbrace{(\theta - \theta_0)}_{\text{Must scale as } 1/\alpha \ll 1}$$

$\gg 1$

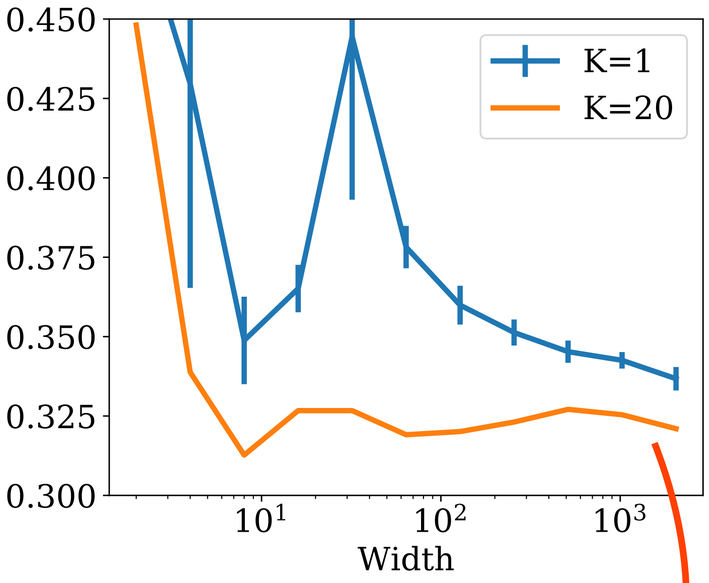
Hence we expect to observe the phase transition of the bias in neural networks at high α

LAZY REGIME OF NEURAL NETWORKS

5-layer MLP on binary 10-PCA CIFAR-10



$\alpha = 10$

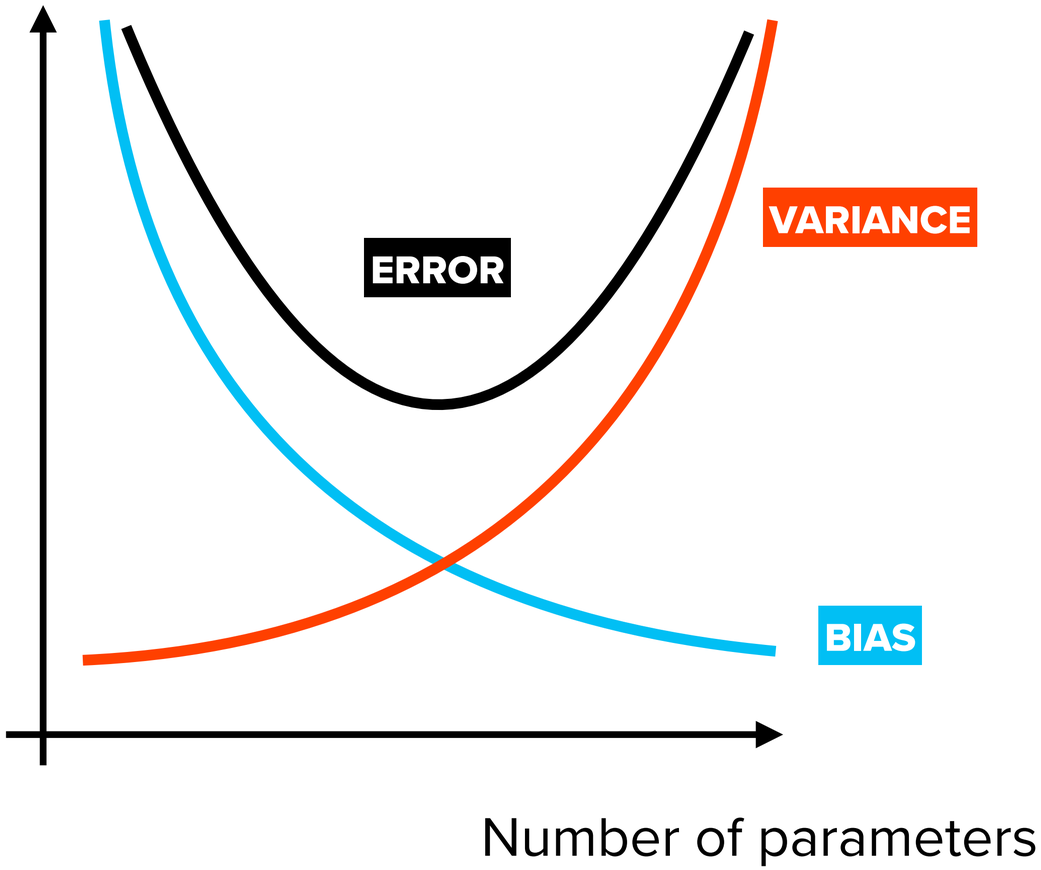


$\alpha = 100$

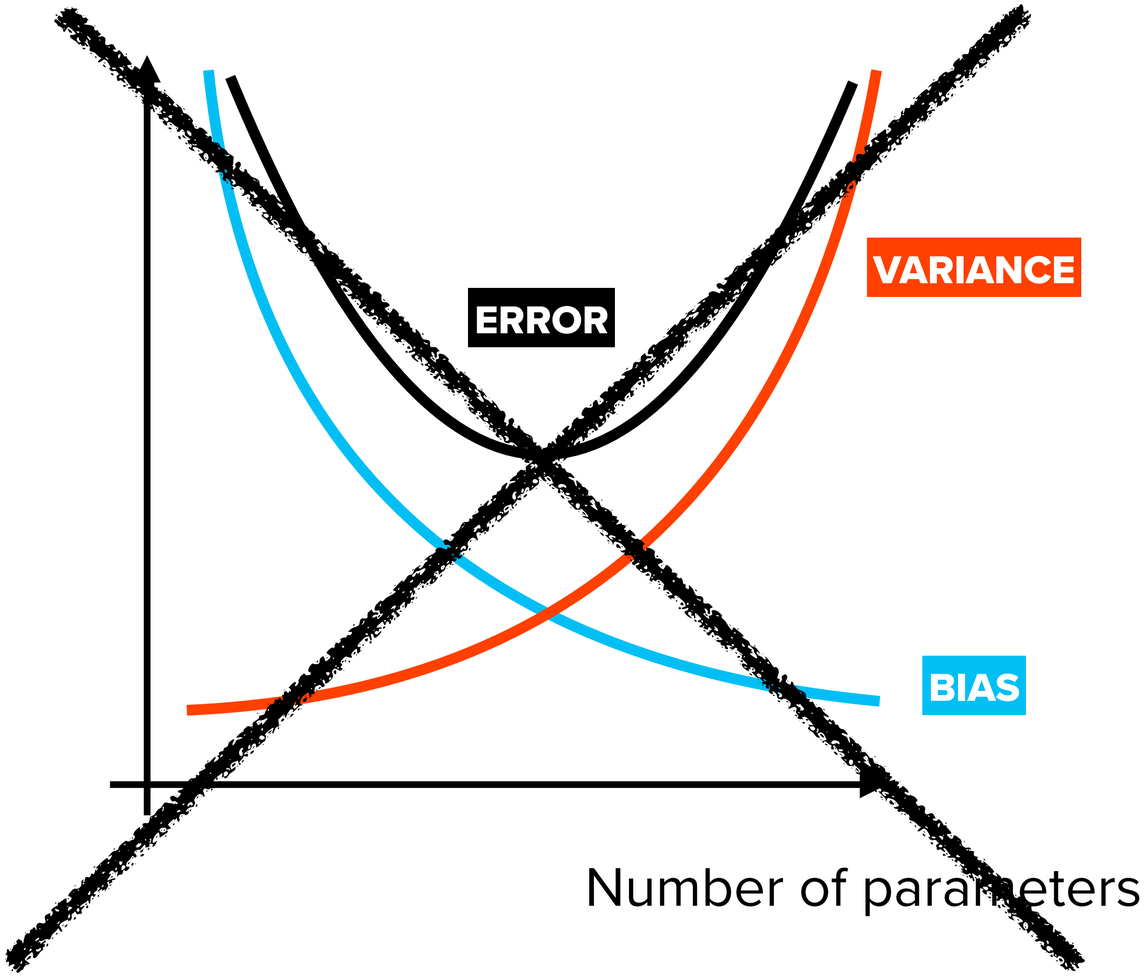
Ensembled error increases
(transition from feature learning to lazy learning)

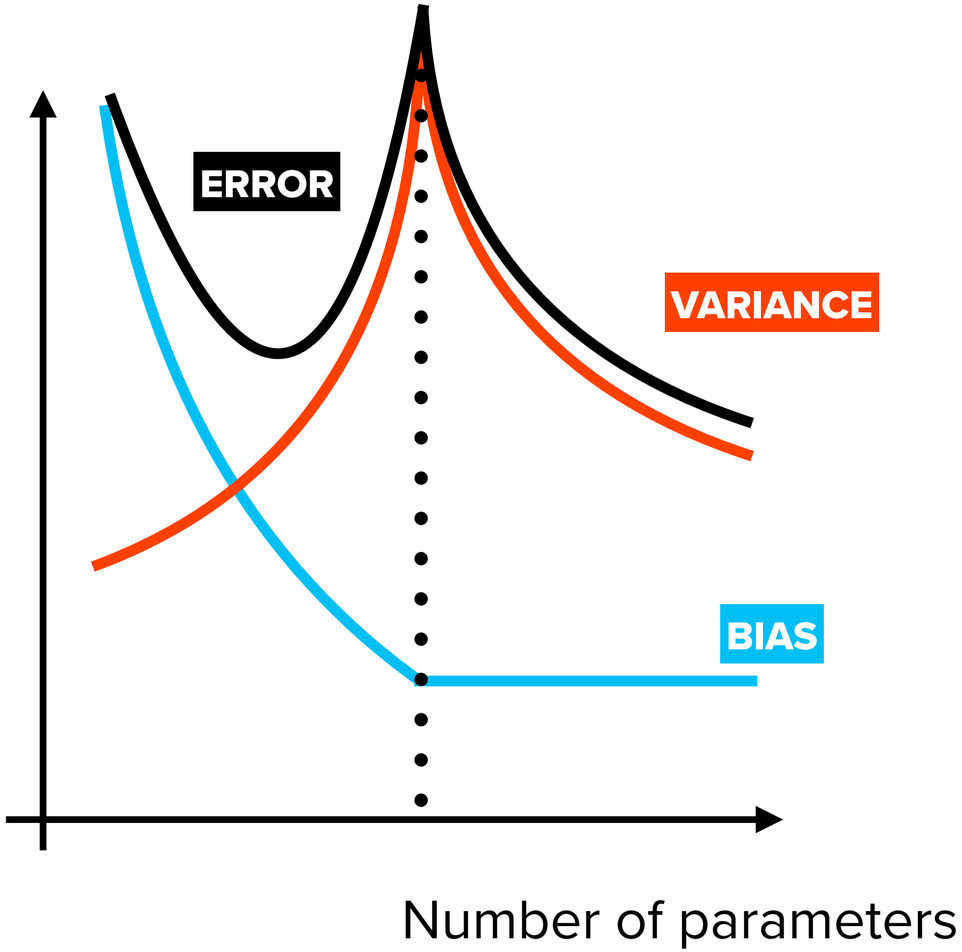
Ensembled error stays flat after interpolation threshold

TAKEAWAY



TAKEAWAY


ERROR
VARIANCE
BIAS
Number of parameters


ERROR
VARIANCE
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THANK YOU FOR YOUR ATTENTION

Stéphane d’Ascoli

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Giulio Biroli

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