

MACHINE LEARNING IN BIOINFORMATICS

MODEL SELECTION AND REGULARIZATION

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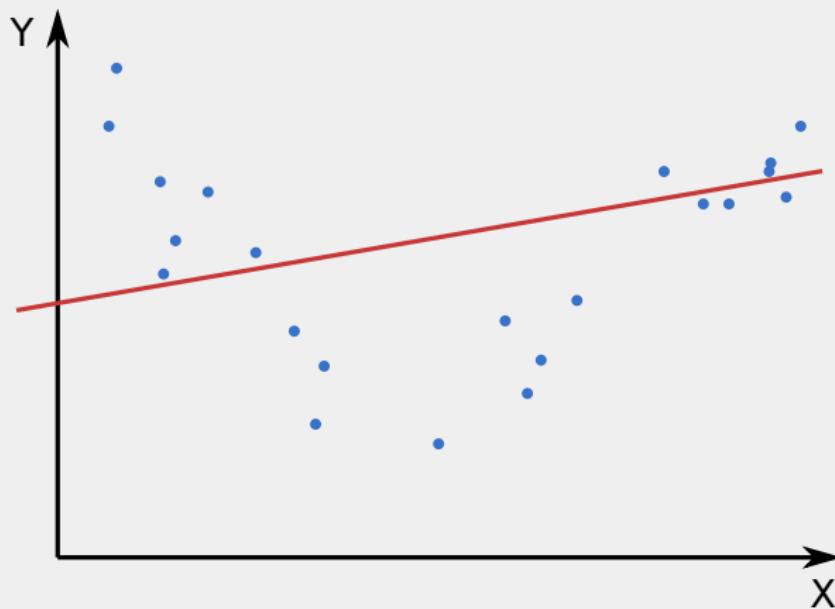
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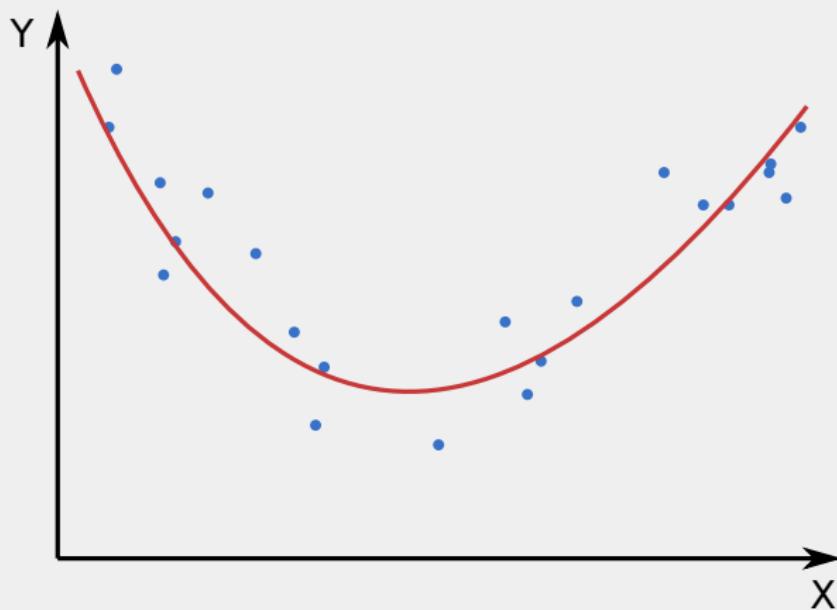
MODEL SELECTION PROBLEM

MODEL SELECTION



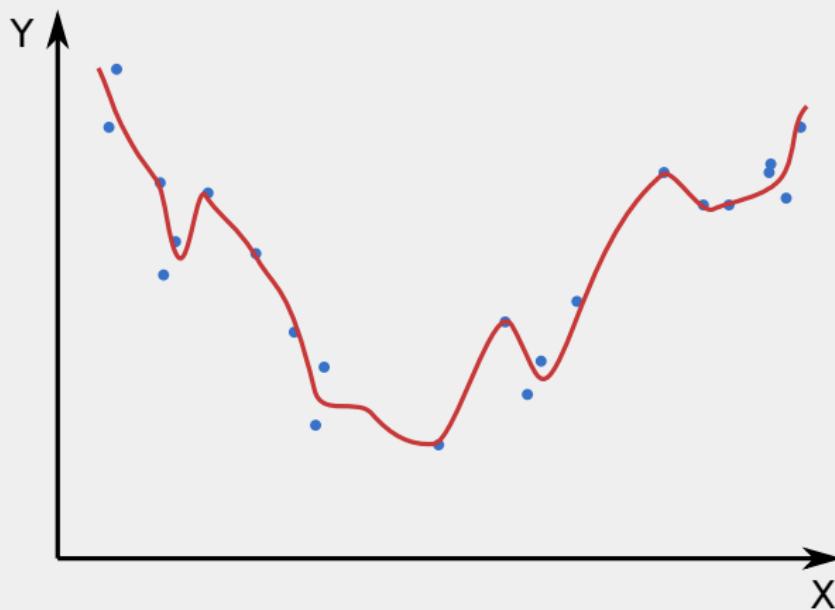
Linear model class

MODEL SELECTION



Quadratic model class

MODEL SELECTION



Polynomial model class

BIAS-VARIANCE DECOMPOSITION AND TRADEOFF

BIAS-VARIANCE DECOMPOSITION

- Let \mathbf{Y} , \mathbf{X} and ϵ be random variables such that $\mathbf{Y} = f(\mathbf{X}) + \epsilon$, with $\mathbb{E}[\epsilon] = 0$ and $\text{var}[\epsilon] = \sigma^2$
- Assume that \hat{f}_D has been estimated on some training data $D = (X, y)$, where X is a matrix of n observations from \mathbf{X} and y a vector of n observations from \mathbf{Y}
- Let $\bar{f}(x) = \mathbb{E}_D[\hat{f}_D(x)]$, then at a query point x we have

$$\mathbb{E}_{\mathbf{Y}, D}[(\mathbf{Y} - \hat{f}_D(x))^2] = \underbrace{[\bar{f}(x) - f(x)]^2}_{\text{Bias}^2} + \underbrace{\mathbb{E}_D[\bar{f}(x) - \hat{f}_D(x)]^2}_{\text{Variance}} + \sigma^2$$

- bias: Is there a bias towards a particular kind of solution (e.g. linear model)? (inductive bias)
- variance: How much does the estimated model change if you train on a different data set? (overfitting)

BIAS-VARIANCE DECOMPOSITION: DERIVATION I

- We study the mean squared prediction error at a fixed x :

$$\mathbb{E}_{\mathbf{Y}, D} [(\mathbf{Y} - \hat{f}_D(x))^2]$$

where $\mathbf{Y} = f(x) + \epsilon$, $\mathbb{E}[\epsilon] = 0$, $\text{Var}(\epsilon) = \sigma^2$.

- **Step 1 – Substitute:**

$$\mathbb{E}_{\epsilon, D} [(f(x) + \epsilon - \hat{f}_D(x))^2]$$

- **Step 2 – Add and subtract the average prediction:**

$$f(x) + \epsilon - \hat{f}_D(x) = \underbrace{(f(x) - \bar{f}(x))}_{\text{bias term}} + \underbrace{(\bar{f}(x) - \hat{f}_D(x))}_{\text{variance term}} + \underbrace{\epsilon}_{\text{noise term}}$$

- **Step 3 – Square and take expectations:** Cross terms vanish because:

BIAS-VARIANCE DECOMPOSITION: DERIVATION II

- ▶ ϵ has mean 0 and is independent of $\hat{f}_D(x)$
- ▶ $\bar{f}(x) - \hat{f}_D(x)$ has mean 0 by definition

■ Result:

$$\begin{aligned}\mathbb{E}_{Y,D}[(Y - \hat{f}_D(x))^2] &= \underbrace{[\bar{f}(x) - f(x)]^2}_{\text{bias}^2} + \underbrace{\mathbb{E}_D[(\bar{f}(x) - \hat{f}_D(x))^2]}_{\text{variance}} + \underbrace{\sigma^2}_{\text{noise}} \\ &\quad + \cancel{\mathbb{E}_D[2(f(x) - \bar{f}(x))(\bar{f}(x) - \hat{f}_D(x))]} \\ &\quad + \cancel{[2(f(x) - \bar{f}(x))\epsilon]} \\ &\quad + \cancel{\mathbb{E}_D[2(\bar{f}(x) - \hat{f}_D(x))\epsilon]} \\ &= (\text{bias})^2 + \text{variance} + \text{noise}.\end{aligned}$$

ESTIMATION ERROR VS. PREDICTION ERROR

■ Estimation Error:

- ▶ Goal: Estimate an unknown fixed quantity (e.g., parameter θ) based on data
- ▶ Decomposition of expected error:

$$\mathbb{E}_X \left[\|\hat{\theta}(X) - \theta\|^2 \right] = \text{Bias}^2 + \text{Variance}$$

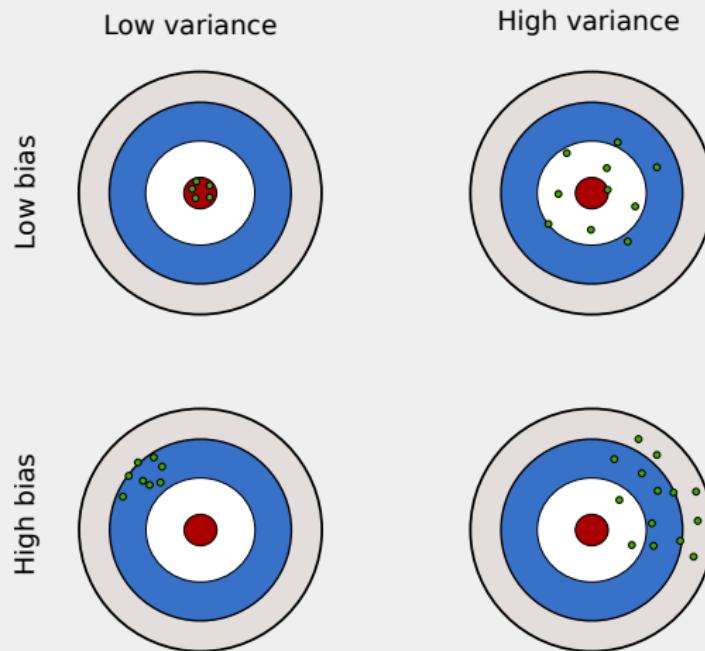
■ Prediction Error:

- ▶ Goal: Predict a future or unseen outcome Y from input X , based on a learned model \hat{f}
- ▶ Decomposition of expected prediction error:

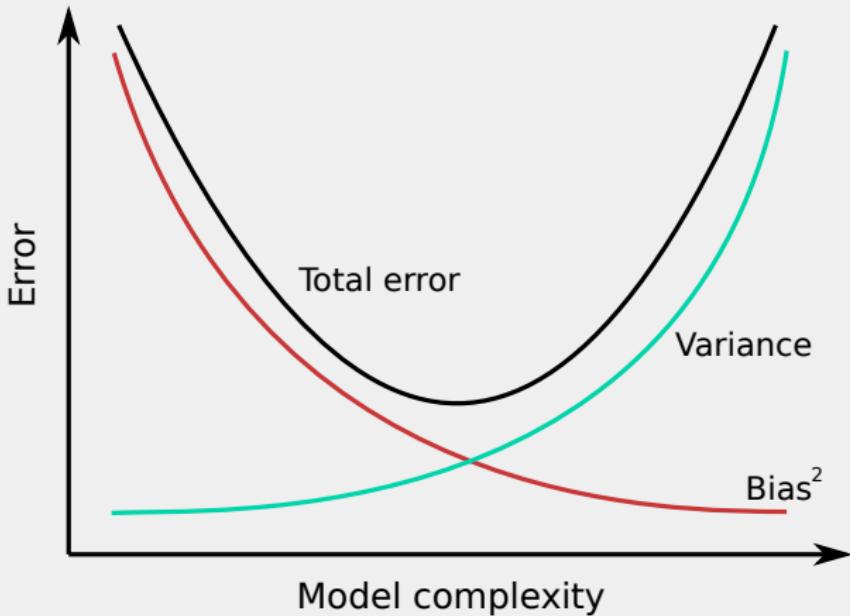
$$\mathbb{E}_{Y,D} \left[(\mathbf{Y} - \hat{f}_D(x))^2 \right] = \text{Bias}^2 + \text{Variance} + \sigma^2$$

- ▶ σ^2 : Irreducible noise from inherent randomness in the data

BIAS-VARIANCE DECOMPOSITION

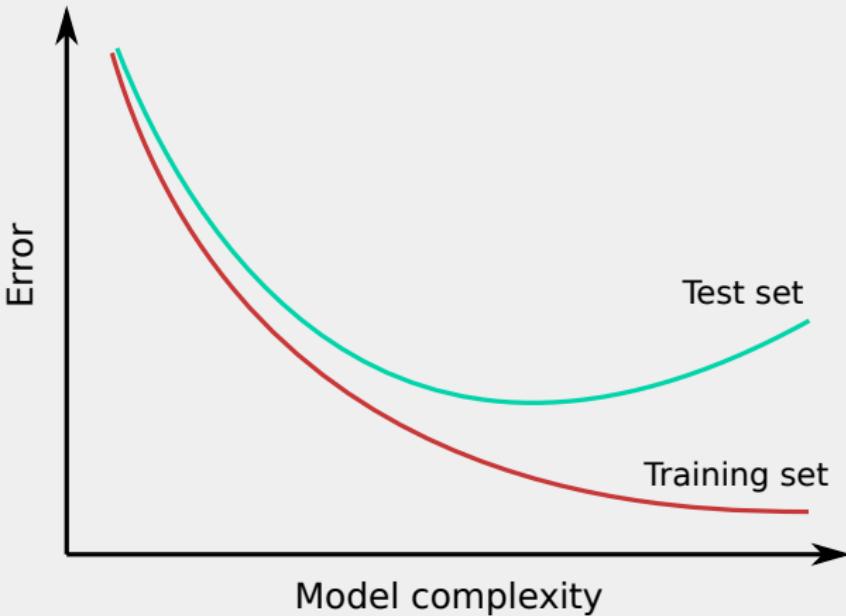


BIAS-VARIANCE DECOMPOSITION



° Note that here we average over multiple data sets. On a single data set we might observe bumps when increasing model complexity

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BIAS-VARIANCE DECOMPOSITION - LESSONS LEARNED

- Every model comes with a bias
- More complex models have a smaller bias but larger variance
- A bias is required to reduce the variance, but introducing a good bias requires domain knowledge
- Classical statistics often uses unbiased estimators, which is nowadays often questioned
- Keep in mind: There is no free lunch!¹

¹The *no free lunch theorem* [Wolpert and Macready, 1997] tells us that there exists no generic model that works well on all domains, but we need to tailor our models to the data at hand in order to introduce a model bias, which reduces variance.

JAMES STEIN ESTIMATOR

THE ESTIMATION PROBLEM

We observe a random vector:

$$X = (\theta_1 + \varepsilon_1, \dots, \theta_p + \varepsilon_p), \quad \varepsilon_i \sim \mathcal{N}(0, \sigma^2)$$

- Each component X_i is a single noisy observation of θ_i
- Only **one observation per dimension** - no replication
- Goal: Estimate the unknown mean vector $\theta = (\theta_1, \dots, \theta_p)$

THE ESTIMATION PROBLEM

- Observations: $X_i \sim \mathcal{N}(\theta_i, \sigma^2)$, independently for $i = 1, \dots, p$
- The likelihood of θ given X is:

$$L(\theta; X) \propto \exp\left(-\frac{1}{2\sigma^2} \|X - \theta\|^2\right)$$

- Maximizing the likelihood \Rightarrow *Maximum Likelihood Estimator (MLE)*:

$$\hat{\theta}_{\text{MLE}} = X$$

EVALUATING ESTIMATORS

Evaluating Estimators: Squared Error Loss

To quantify how well an estimator performs, we use the loss function:

$$L(\hat{\theta}, \theta) = \|\hat{\theta} - \theta\|^2$$

and define its **risk** (expected loss):

$$R(\hat{\theta}, \theta) = \mathbb{E}_{\theta} \left[\|\hat{\theta}(X) - \theta\|^2 \right]$$

- Under squared error loss, the risk can be decomposed into:

$$\text{Risk} = \|\text{Bias}(\hat{\theta})\|^2 + \text{Var}(\hat{\theta})$$

- This bias-variance decomposition helps us understand tradeoffs in estimator performance.

EVALUATING ESTIMATORS

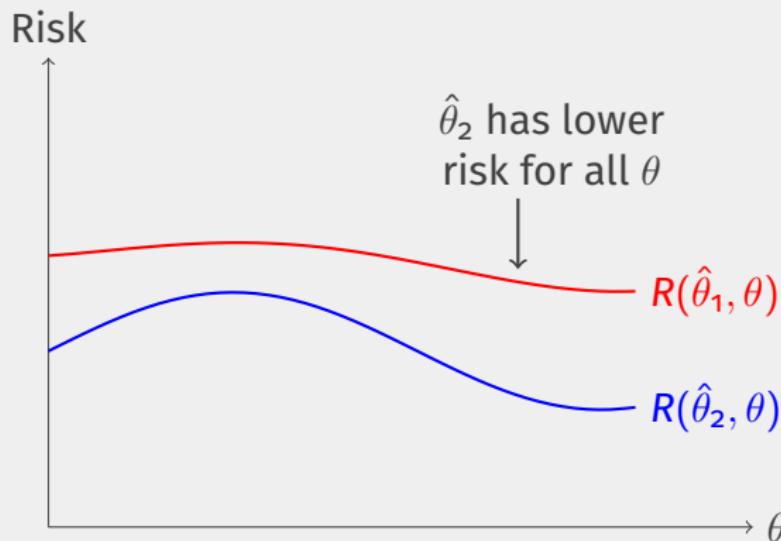
Risk and Admissibility

- The **risk** of an estimator is its expected loss:

$$R(\hat{\theta}, \theta) = \mathbb{E}_{X \sim P_\theta} \left[\|\hat{\theta}(X) - \theta\|^2 \right]$$

- An estimator is **admissible** if no other estimator has uniformly lower risk (i.e., lower for all θ , strictly lower for some).

EVALUATING ESTIMATORS



- An estimator that is tuned to perform best at a specific parameter value can have very low risk at that point, but much higher risk elsewhere.

SURPRISING RESULT

James–Stein Theorem [James et al., 1961]

For $p \geq 3$, the MLE $\hat{\theta}_{\text{MLE}} = X$ is **inadmissible** under squared error loss.

- There exists an estimator with strictly lower risk than the MLE for all θ
- This result shocked statisticians: the unbiased estimator is not optimal!

JAMES-STEIN ESTIMATOR

The James–Stein estimator is defined as:

$$\hat{\theta}_{JS} = \left(1 - \frac{(p-2)\sigma^2}{\|X\|^2}\right) X$$

- Shrinks X toward the origin
- Introduces bias, but reduces variance
- Dominates MLE in risk for $p \geq 3$

POSITIVE-PART JAMES-STEIN ESTIMATOR

To avoid over-shrinking:

$$\hat{\theta}_{JS}^+ = \left(1 - \frac{(p-2)\sigma^2}{\|X\|^2} \right)_+ X$$

where $(a)_+ = \max(a, 0)$

- Further reduces risk
- Dominates the standard James-Stein estimator
- Still inadmissible, but better performance

KEY TAKEAWAYS I

- We observe one noisy measurement per parameter:
 $X_i \sim \mathcal{N}(\theta_i, \sigma^2)$
- As dimension p increases, the number of parameters increases – but the information per parameter stays the same
- The MLE is unbiased but has high variance in high dimensions
- Shrinkage estimators (like James–Stein) reduce variance at the cost of bias, improving overall estimation
- Bayes and empirical Bayes estimators can be admissible and offer further improvement

KEY TAKEAWAYS II

Conclusion

Without regularization, estimating many parameters from few observations leads to poor performance.

Historical Impact [Efron and Morris, 1977]

In 1961, the maximum likelihood estimator (MLE) was widely believed to be the best estimator one could hope for, especially if it was unbiased. James and Stein's theorem showed that for $p \geq 3$, the MLE is **inadmissible** under squared error loss: there exists another estimator with strictly lower risk for all θ . This surprising result revolutionized statistical thinking and inspired the development of shrinkage methods, empirical Bayes, and modern regularization techniques.

WHICH ESTIMATOR IS ADMISSIBLE? I

- The MLE, James–Stein, and positive-part James–Stein estimators are all **inadmissible** (in sufficiently high dimension).
- **Admissible:** No other estimator has uniformly lower risk (lower for all θ , strictly lower for some).

WHICH ESTIMATOR IS ADMISSIBLE? II

Admissibility of Bayes Estimator

[Berger, 2013, Lehmann and Casella, 1998]

Let $\pi(\theta)$ be any **proper** prior distribution and consider squared error loss:

$$L(\hat{\theta}, \theta) = \|\hat{\theta} - \theta\|^2.$$

Then the Bayes estimator

$$\hat{\theta}_{\text{Bayes}}(x) = \mathbb{E}[\theta | X = x]$$

is **admissible**.

- Admissibility means no other estimator dominates it uniformly, but does *not* imply low risk for all θ .

WHICH ESTIMATOR IS ADMISSIBLE? III

- If the prior is concentrated far from the true θ , the estimator may have low risk near the prior mean but high risk elsewhere.
- **Example:** For $\theta \sim \mathcal{N}(\mu_0, \tau^2 I_p)$ and $X | \theta \sim \mathcal{N}(\theta, \sigma^2 I_p)$,

$$\hat{\theta}_{\text{Bayes}} = \mu_0 + \frac{\tau^2}{\tau^2 + \sigma^2} (X - \mu_0)$$

is admissible for any $\tau^2 > 0$. Small τ^2 causes strong shrinkage toward μ_0 .

- The degenerate case $\tau^2 = 0$ is not a proper prior and admissibility is not guaranteed.

COMPLEXITY MEASURES

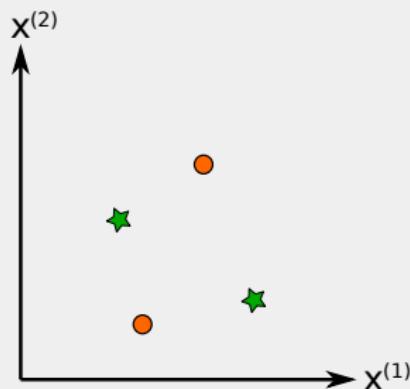
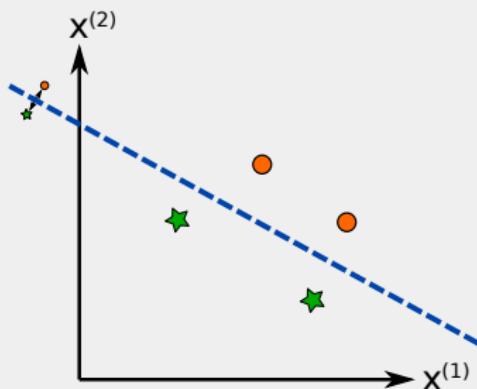
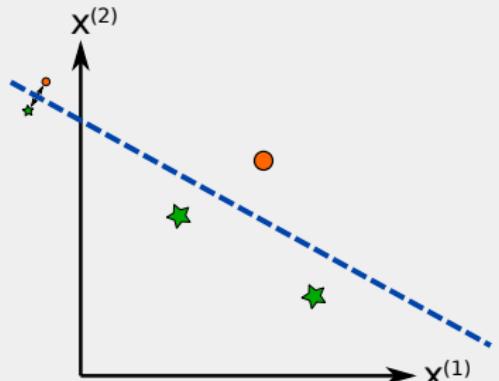
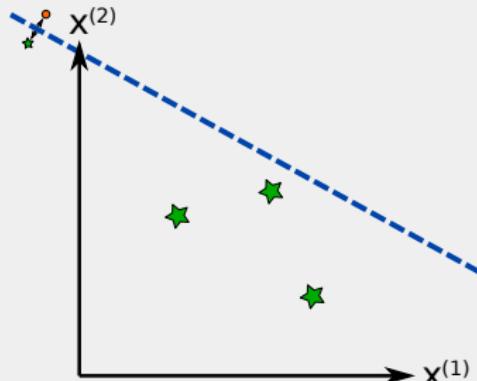
VC-Dimension (Vapnik Chervonenkis)

Let \mathbb{F}_p be a set of classifiers on an n -dimensional input space. The VC-dimension $\text{VC}(\mathbb{F}_p)$ is defined as the maximum number of points that can be correctly classified by at least one member of \mathbb{F}_p .

■ Examples:

- ▶ Linear classifier on \mathbb{R}^p : $\text{VC} = p + 1$
- ▶ SVM with RBF kernel: $\text{VC} = \infty$
- ▶ Neural network with n_e edges, n_v nodes and sigmoid activation function: $\Omega(n_e^2) < \text{VC} < \mathcal{O}(n_e^2 n_v^2)$
[Shalev-Shwartz and Ben-David, 2014, Section 20.4]

COMPLEXITY OF CLASSIFIERS - VC DIMENSION



MEASURES OF MODEL COMPLEXITY - DF

Degrees of Freedom (DF) [Efron, 1986]

The **degrees of freedom** of an estimate $\hat{y} = \hat{f}(X)$ is defined as

$$\text{df}(\hat{y}) = \frac{1}{\sigma^2} \sum_{i=1}^n \text{cov}(\hat{y}_i, y_i) = \frac{1}{\sigma^2} \text{tr cov}(\hat{y}, y),$$

where

- X denotes a fixed set of n covariates of dimension p
- $y = (y_1, \dots, y_n)$ is a vector of n observations from

$$\mathbf{Y} = f(X) + \epsilon$$

for some function f , assuming $\mathbb{E}[\epsilon] = 0$ and $\text{var}[\epsilon] = \sigma^2$

¹df is normalized by the magnitude of the aleatory uncertainty (σ^2)

MEASURES OF MODEL COMPLEXITY - DF

- Degrees of freedom for the OLS estimate:

$$\begin{aligned}\text{df}(\hat{y}) &= \frac{1}{\sigma^2} \text{tr cov}(\hat{y}, y) \\ &= \frac{1}{\sigma^2} \text{tr cov} \left(X(X^\top X)^{-1} X^\top y, y \right) \\ &= \frac{1}{\sigma^2} \text{tr} \left(X(X^\top X)^{-1} X^\top \right) \text{cov}(y, y) \\ &= \text{tr} \left(X(X^\top X)^{-1} X^\top \right) \\ &= p\end{aligned}$$

- $\text{df}(\hat{y}) = p$, i.e. the number of parameters, assuming independent feature vectors (i.e. columns of X)
- This result holds for $p < n$

$X(X^\top X)^{-1} X^\top$ is the hat matrix $H \in \mathbb{R}^{n \times n}$, hence $\text{df}(\hat{y}) = \text{rank}(H)$

MEASURES OF MODEL COMPLEXITY - DF

- Ridge regression is defined as

$$\hat{\theta} = \arg \min_{\theta} \|y - X\theta\|_2^2 + \lambda \|\theta\|_2^2$$

for some regularization strength $\lambda \geq 0$

- The ridge estimator has

$$df(\hat{y}) = \sum_{j=1}^p \frac{d_j^2}{d_j^2 + \lambda}$$

degrees of freedom, where $(d_j)_j$ are the singular values of X

- Increasing λ decreases model complexity

MEASURES OF MODEL COMPLEXITY - DF

- There is some criticism about used DF as measure of model complexity [Janson et al., 2015]
- In some cases, we also need X to be random [Luan et al., 2021]
- We will see other measures when turning to model selection

MODEL SELECTION

MODEL SELECTION APPROACHES

- A measure of accuracy or fit, such as the mean squared error (MSE), is not enough: Increasing model complexity will always lead to a better fit
- Estimating a model requires to minimize both
 - ▶ **in-sample-error** (loss on training data), and
 - ▶ **out-of-sample-error** (generalization error)
- Cross-validation (CV) estimates generalization error on left-out samples²
- Traditional statistics: Combine measure of accuracy (in-sample-error) with a penalty for complexity

²Heavy hyperparameter tuning using CV can lead to overfitting and requires to select a final holdout set

MODEL SELECTION APPROACHES - LOO-CV

- Leave-one-out Cross-Validation (LOO-CV) at iteration $i = 1, 2, \dots, n$:
 - ▶ Compute estimate on data set without the i -th sample
 - ▶ Compute prediction error on the i -th sample
- Report the average prediction error over all n samples
- PRESS statistic (predicted residual error sum of squares):

$$\text{PRESS} = \sum_{i=1}^n (y_i - \hat{y}_{-i})^2$$

where \hat{y}_{-i} is the prediction for the i -th sample where the model has been estimated on all but the i -th sample

MODEL SELECTION APPROACHES - PRESS

- LOO-CV is very costly for large data sets and complex models
- k -fold CV with $k = 5$ or $k = 10$ is often used in practice
- For (ridge) linear regression with mean squared error we can efficiently compute LOO-CV [Cook, 1977]

$$\begin{aligned}\text{PRESS} &= \sum_{i=1}^n (y_i - \hat{y}_{-i})^2 \\ &= \sum_{i=1}^n \frac{(y_i - \hat{y}_i)^2}{(1 - H_{ii})^2}\end{aligned}$$

- The matrix

$$H = X(X^\top X + \lambda I)^{-1}X^\top$$

is called the hat matrix, because it puts a hat on y , i.e. $\hat{y} = Hy$

MODEL SELECTION APPROACHES - GCV

- Models like smoothing splines or kernel regressions still have a hat matrix, but it is costly or undefined in closed form.
- H may be dense, very large, or not explicitly known.
- Generalized Cross-Validation (GCV) uses the approximation

$$H_{ii} \approx \text{tr}(H)/n$$

- The GCV therefore is defined as

$$\text{GCV} = \frac{\|y - \hat{y}\|^2}{\left(1 - \frac{\text{tr}(H)}{n}\right)^2}$$

- GCV only requires $\text{tr}(H)$, which can often be approximated (e.g. using randomized trace estimation).

MODEL SELECTION APPROACHES

- LOO-CV is computationally very expensive
- k -fold CV is cheaper, but uses a large fraction of the data for testing
- Model performance could be better if this data was used for training
- Overfitting if we use CV for testing too many models (requires final hold out data)
- **Can we do model selection by using all data for training?**

MODEL SELECTION APPROACHES - DF

- Assume again the following model

$$\mathbf{Y} = f(\mathbf{X}) + \epsilon$$

where $\mathbf{X} \in \mathbb{R}^{n \times p}$ is a fixed set of n predictors and $\mathbf{Y} \in \mathbb{R}^n$

- Setup is very similar to the bias-variance decomposition, but X is now fixed
- Let $\mathbf{Y}_t \in \mathbb{R}^n$ a vector of n independent observations and $\hat{f}_{\mathbf{Y}_t}$ an estimate on the training set $(\mathbf{X}, \mathbf{Y}_t)$, then [Efron, 1986]

$$\underbrace{\mathbb{E}_{\mathbf{Y}, \mathbf{Y}_t} \left\| \mathbf{Y} - \hat{f}_{\mathbf{Y}_t}(\mathbf{X}) \right\|_2^2}_{\text{expected prediction error}} = \underbrace{\mathbb{E}_{\mathbf{Y}_t} \left\| \mathbf{Y}_t - \hat{f}_{\mathbf{Y}_t}(\mathbf{X}) \right\|_2^2}_{\text{expected training error}} + 2\sigma^2 \text{df}(\hat{f})$$

MODEL SELECTION APPROACHES - DF

- This motivates the following model selection criterium [Mallows, 2000]

$$\underbrace{\left\| y_t - \hat{f}_{y_t}(X) \right\|_2^2}_{\text{training error}} + \underbrace{2\sigma^2 \text{df}(\hat{f})}_{\text{complexity penalty}}$$

- The more complex a model, the larger the penalty
- If two models fit the data equally well, we select the simpler one (Occam's razor)

MODEL SELECTION APPROACHES - BAYES APPROACH

- Assume we have a set of models $(m_i)_i$
- In a probabilistic setting we evaluate the probability of a model m_i given data x , i.e. using Bayes theorem

$$\text{pr}(m_i | x) = \frac{\text{pr}(x | m_i)\text{pr}(m_i)}{\sum_j \text{pr}(x | m_j)\text{pr}(m_j)} = \frac{\text{pr}(x | m_i)\text{pr}(m_i)}{\text{pr}(x)}$$

- We compare two models m_i and m_j using

$$\frac{\text{pr}(m_i | x)}{\text{pr}(m_j | x)} = \frac{\frac{\text{pr}(x | m_i)\text{pr}(m_i)}{\text{pr}(x)}}{\frac{\text{pr}(x | m_j)\text{pr}(m_j)}{\text{pr}(x)}} = \frac{\text{pr}(x | m_i)\text{pr}(m_i)}{\text{pr}(x | m_j)\text{pr}(m_j)}$$

because $\text{pr}(x)$ drops

MODEL SELECTION APPROACHES - BAYES FACTOR

- With a uniform prior over models we arrive at the Bayes factor [Kass and Raftery, 1995]

$$\frac{\text{pr}(x | m_i)}{\text{pr}(x | m_j)}$$

- Hence, in Bayesian model selection, we evaluate a model m based on its *marginal likelihood*

$$\text{pr}(x | m) = \int_{\theta} \text{pr}(x | \theta, m) \text{pr}(\theta | m) d\theta$$

where θ are the model parameters

- The marginal likelihood is often difficult to evaluate, even numerically!

MODEL SELECTION APPROACHES - BIC

- The marginal likelihood is tractable only for very simple models
- As an alternative, we use approximations of the marginal likelihood
- The **Bayes information criterion (BIC)** is such an approximation. Let x contain n samples and assume that $n \gg p$, then

$$\text{pr}(x | m) \approx \exp \left\{ -\frac{1}{2} \text{BIC}(x; m) \right\}$$

$$\text{BIC}(x; m) = -2 \log \text{pr}(x | \hat{\theta}, m) + p \log(n)$$

where $\hat{\theta}$ refers to the maximum likelihood estimate and p to the number of parameters

MODEL SELECTION APPROACHES - BIC

- Let \mathbf{Y} and ϵ be two random variables such that $\mathbf{Y} = f(X) + \epsilon$
- Let $f_{\hat{\theta}}$ denote a maximum likelihood estimate on some training data
- For $\epsilon \sim \text{Normal}(0, \sigma^2)$ the BIC is related to the mean squared error with complexity penalty

$$\begin{aligned}\text{BIC}(x; m) &= \frac{1}{\sigma^2} \sum_{i=1}^n (y_i - f_{\hat{\theta}}(x_i))^2 + p \log(n) + C_n \\ &\propto \frac{1}{\sigma^2} \|y - f_{\hat{\theta}}(x)\|_2^2 + p \log(n)\end{aligned}$$

where C_n is a constant depending on n , which can be dropped for model comparison

MODEL SELECTION APPROACHES - FIC

- BIC assumes $n \gg p$ and therefore depends only on the number of parameters
- Fisher Information Approximation (FIA) [Ly et al., 2017]:

$$\text{pr}(x | m) \approx \exp \{-\text{FIA}(x; m)\}$$

$$\text{FIA}(x; m) = \underbrace{-\log \text{pr}(x | \hat{\theta}, m)}_{\text{BIC like term}} + \frac{p}{2} \log \left(\frac{n}{2\pi} \right) + \log C_m$$

$$C_m = \underbrace{\int_{\theta} \sqrt{\det \mathcal{I}_m(\theta)} d\theta}_{\text{Geometric complexity}}$$

where \mathcal{I}_m denotes the *Fisher information matrix*

- C_m is essential if $n \gg p$ is not given
[Cheema and Sugiyama, 2020]

HOW DO WE CONTROL MODEL COMPLEXITY?

- Regularization (e.g. ridge regression):
 - ▶ Constrain the feasible set of parameter values
 - ▶ Keep the number of parameters in the model constant, but allow them to become zero
- Number of parameters:
 - ▶ A good approximation of model complexity if $n > p$
 - ▶ For $n < p$ we saw that the optimization problem has many solutions
 - In deep neural networks, the gradient descent method can act similar to a regularizer
 - Model complexity can decrease when adding more parameters (double descent)

REGULARIZATION

ℓ_k -PENALIZED REGRESSION

Objective function

$$\omega(\theta) = -\log \text{pr}_\theta(y) \quad (\text{maximum likelihood}), \text{ or}$$

$$\omega(\theta) = \|y - X\theta\|_2^2 \quad (\text{linear regression})$$

Regularized estimate with ℓ_k -norm penalty

$$\hat{\theta} = \begin{cases} \arg \min_{\theta} & \omega(\theta) \\ \text{subject to} & \|\theta\|_k^k = \Lambda \end{cases}$$

where

$$\|\theta\|_k = \left(\sum_{j=2}^p |\theta_j|^k \right)^{1/k}$$

²Remember that we do not regularize the bias or y-intercept θ_0

l_k -PENALIZED REGRESSION

Identify saddle points of Lagrangian

$$\mathcal{L}(\theta, \lambda) = \omega(\theta) + \lambda(\|\theta\|_k^k - \Lambda)$$

In practice, we do not work with Λ , but set λ such that the classification performance is optimal, i.e. we work with the Lagrangian

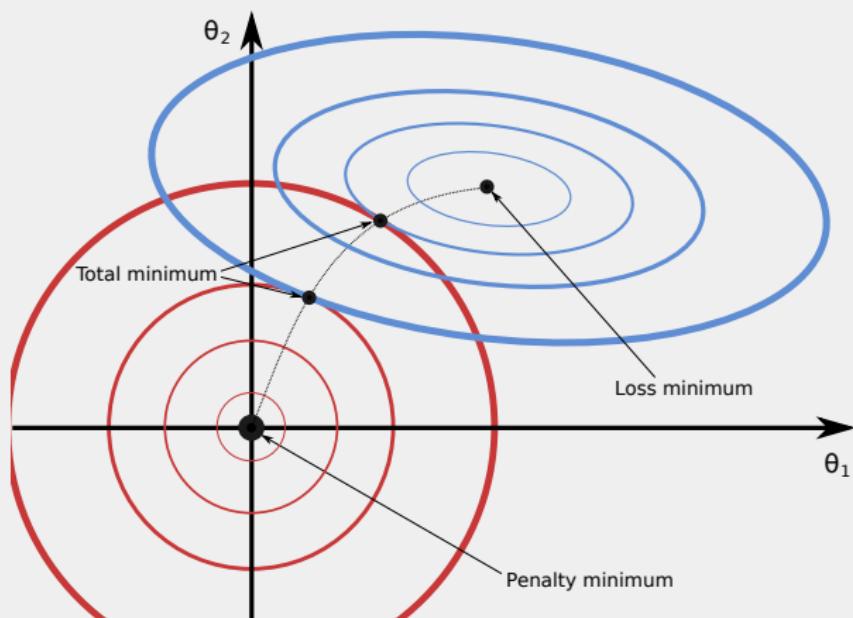
$$\hat{\theta}(\lambda) = \arg \min_{\theta} \omega(\theta) + \lambda \|\theta\|_k^k$$

At the optimum we must have

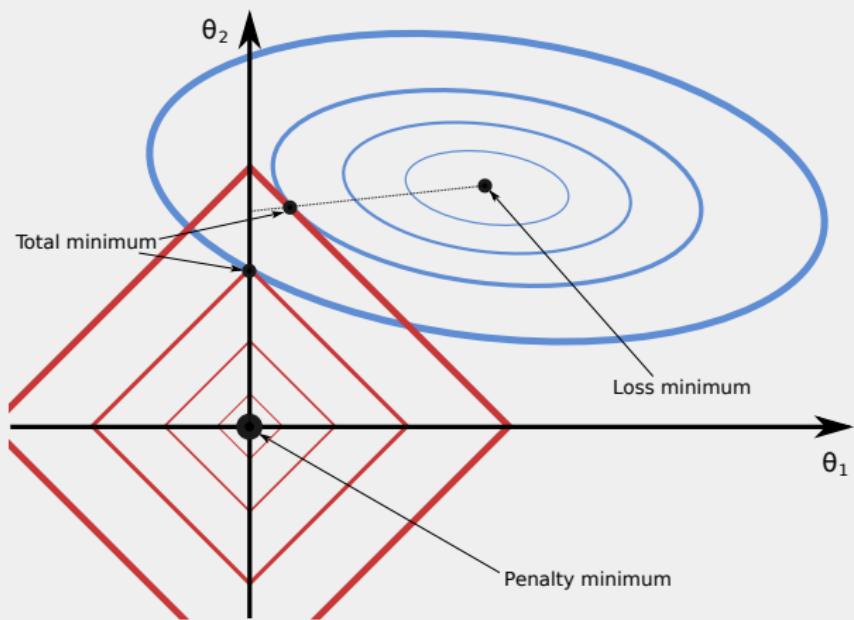
$$\nabla_{\theta} \omega(\theta) + \lambda \nabla_{\theta} \|\theta\|_k^k = \mathbf{0}$$

i.e. the gradients of $\omega(\theta)$ and $\lambda \|\theta\|_k^k$ must point to opposite directions

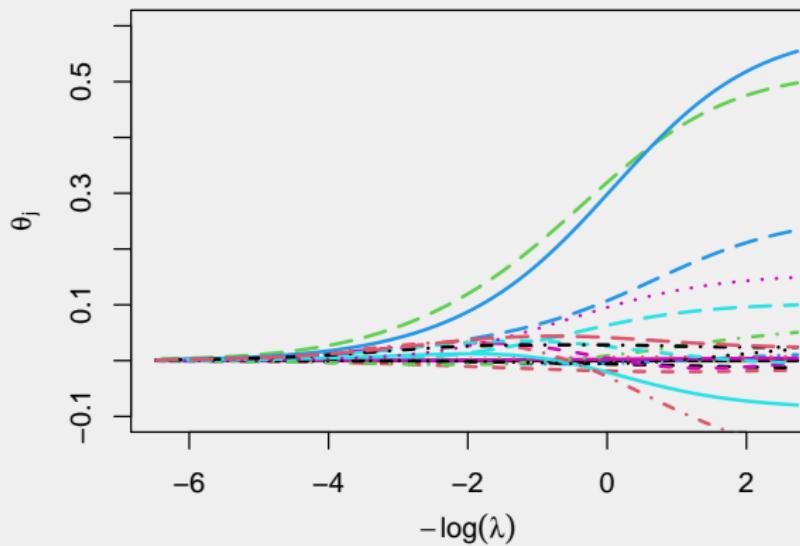
REGULARIZATION - K=2



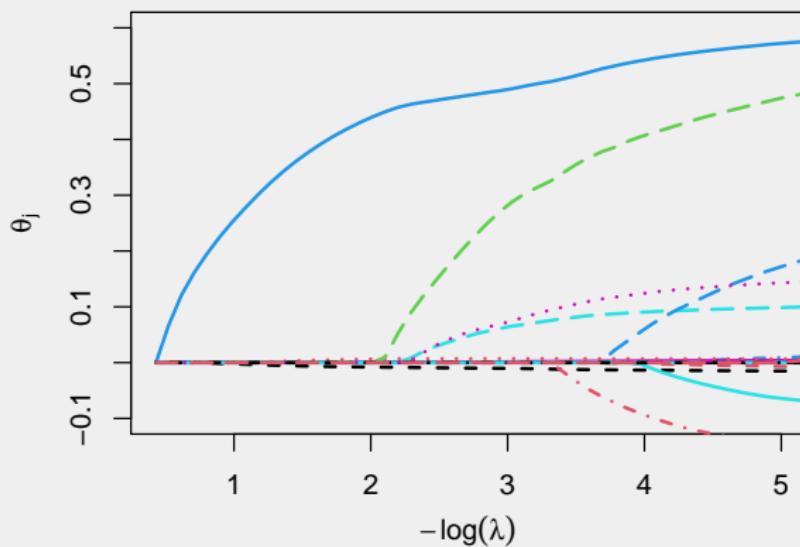
REGULARIZATION - K=1



REGULARIZATION PATHS - K=2

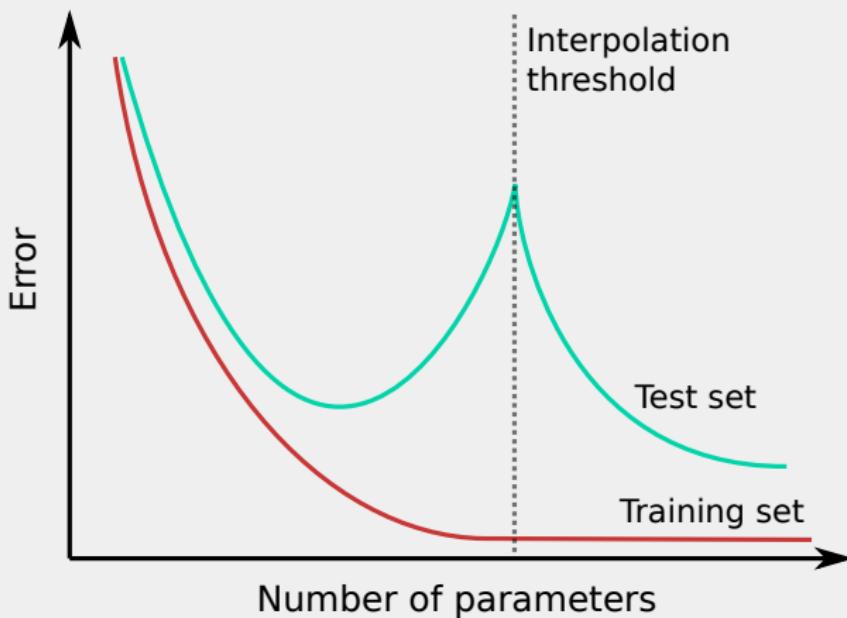


REGULARIZATION PATHS - K=1

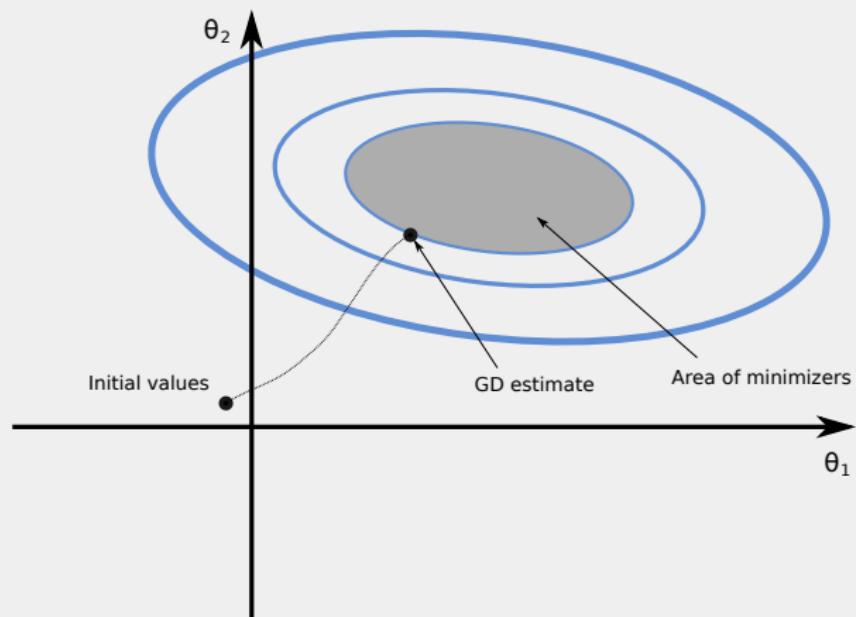


IMPLICIT REGULARIZATION AND DOUBLE DESCENT

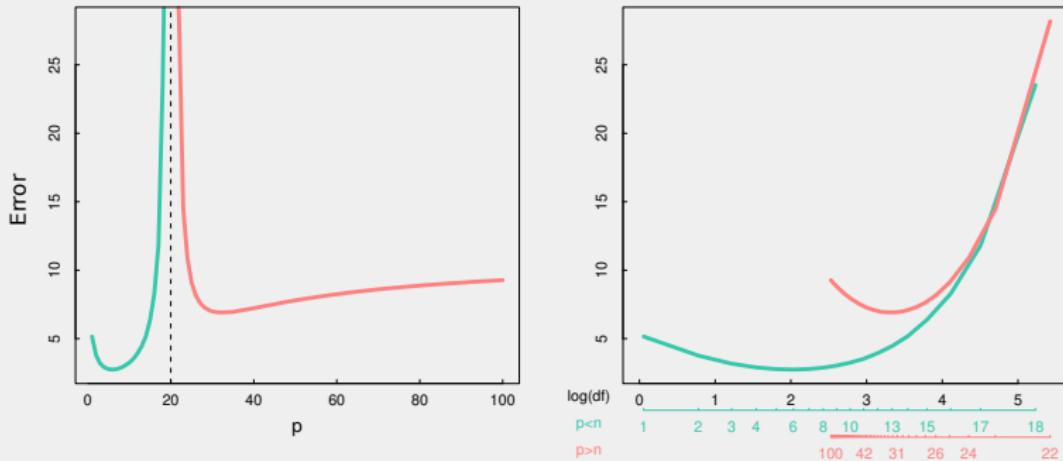
IMPLICIT REGULARIZATION - DOUBLE DESCENT



IMPLICIT REGULARIZATION - DOUBLE DESCENT



MINIMUM ℓ_2 -NORM ESTIMATE - DF



²Requires a more advanced definition of DF that treats X as random variable [Luan et al., 2021]

IMPLICIT REGULARIZATION

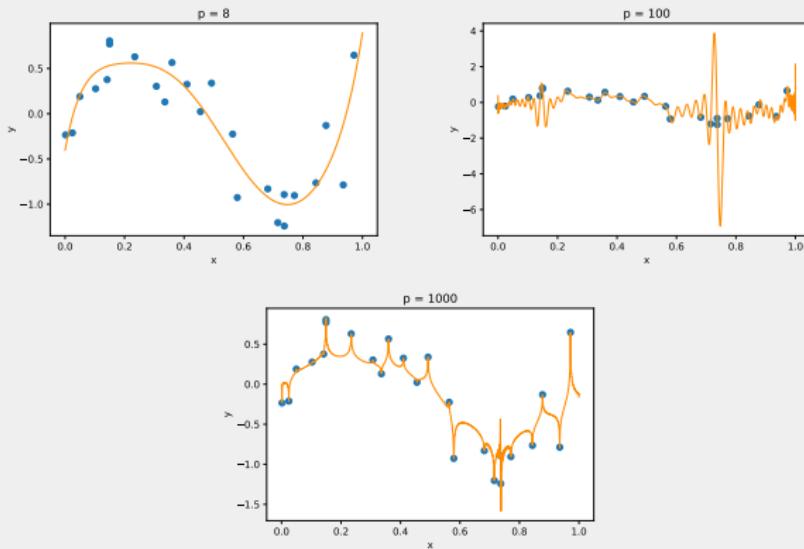


Figure: Fitting degree $d = p - 1$ Legendre polynomials. For $p > n$ the solution with the smallest ℓ_2 -norm is used.

²Legendre polynomials are quite useful, since their absolute value is bounded by one.

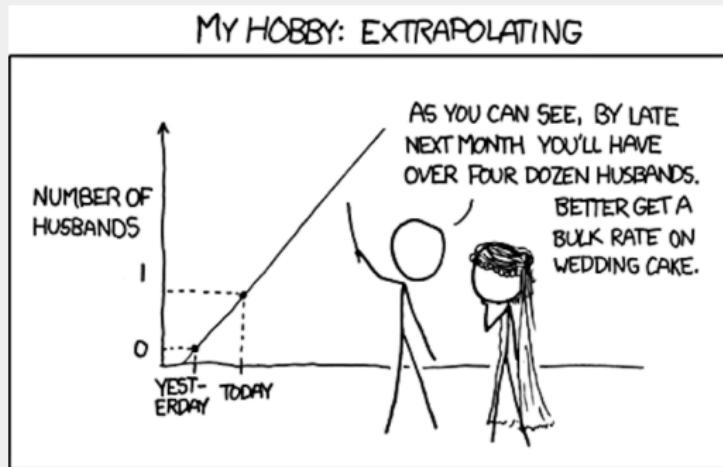
TAKE HOME MESSAGES

- Expected performance is the sum of training performance and model complexity
- Complex models require regularization to prevent overfitting
- The number of parameters does not correspond to the complexity of a model
- Increasing the number of features can reduce model complexity if a min- ℓ_2 -norm estimator is used
- If we have complex data and cannot make any assumptions on the generating process, we might be better off with an overparametrized model using regularization (success behind deep learning)

MORE REFERENCES

- Akaike information criterion (AIC)
[Akaike, 1974, Cavanaugh and Neath, 2019]
- Bayesian information criterion (BIC) [Schwarz, 1978]
- Deviance information criterion (DIC)
[Spiegelhalter et al., 2002]
- Fisher Information Approximation (FIA) [Rissanen, 1996, Grünwald, 2007, Cheema and Sugiyama, 2020]
- Degrees of freedom (DF)
[Tibshirani, 2015, Gao and Jovic, 2016, Luan et al., 2021]
- Implicit regularization and double descent
[Hastie et al., 2022, Luan et al., 2021, Derezhinski et al., 2020, Kobak et al., 2020]

OVERFITTING



READING

- Sections 3.4, 7.3, 7.6, 7.7 and 7.9 [Hastie et al., 2009]

THE END

"All models are wrong, but some are useful."
[Moody, 1991]

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