Machine Learning in Bioinformatics

Model Selection and Regularization

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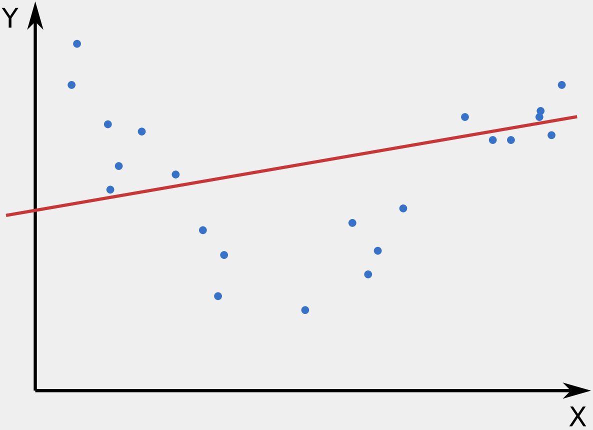
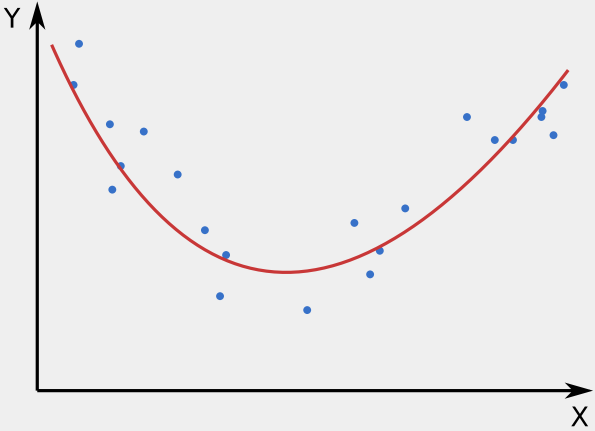
Model selection problem

Model selection



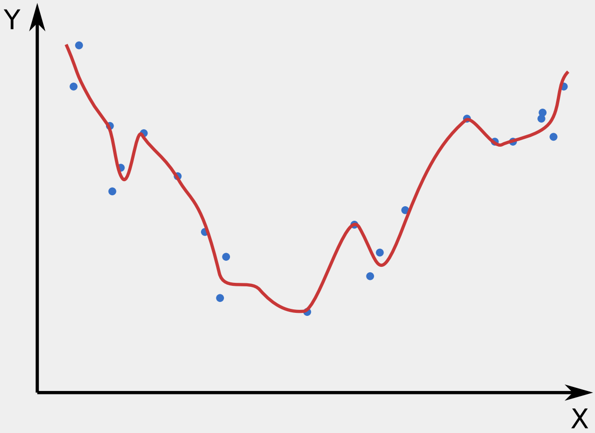
Linear model class

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 $\mathrm{var}[\epsilon] = \sigma^2$

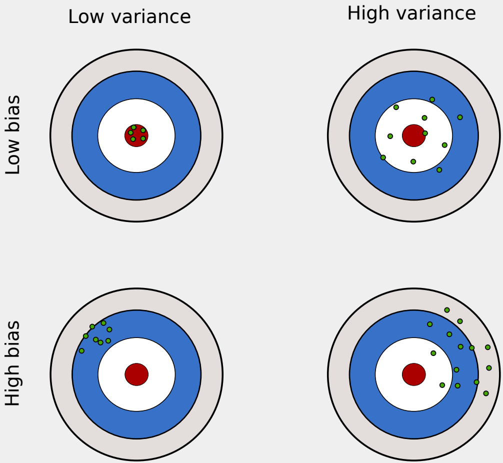
- Assume that $\hat{f}_D$ has been estimated on some training data $D = (X, y)$, where X is a matrix of n observations from $\mathbf{X}$ and y a vector of n observations from $\mathbf{Y}$

- At a query point x we have

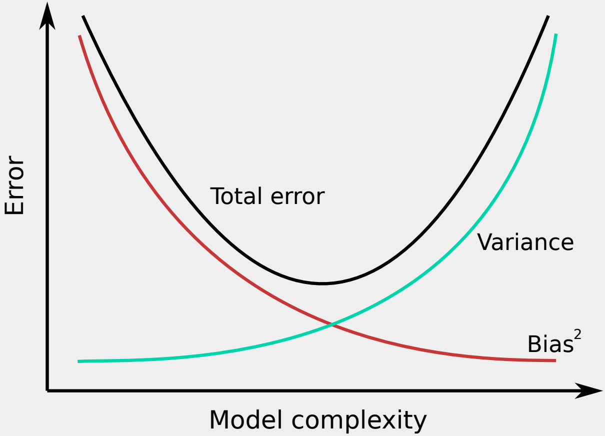
$$\mathbb{E}_{\mathbf{Y},D}[(\mathbf{Y} - \hat{f}_D(x))^2] = \underbrace{[\mathbb{E}_D \hat{f}_D(x) - f(x)]^2}_{\text{Bias}^2} + \underbrace{\mathbb{E}_D[\hat{f}_D(x) - \mathbb{E}_D \hat{f}_D(x)]^2}_{\text{Variance}} + \sigma^2$$

- 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

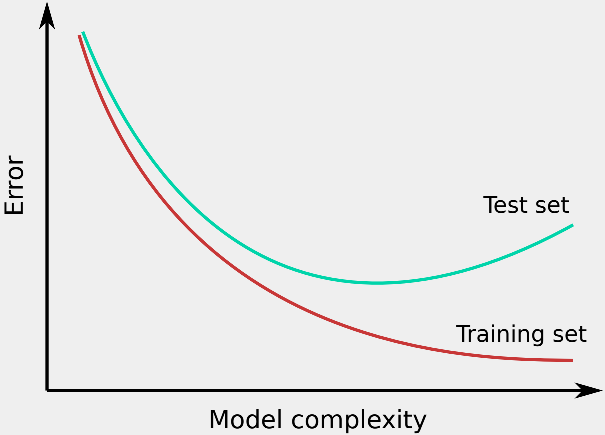


Bias-Variance decomposition



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

Bias-Variance decomposition



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

Bias-Variance decomposition - Lessions 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]

[1] The *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.

Complexity measures

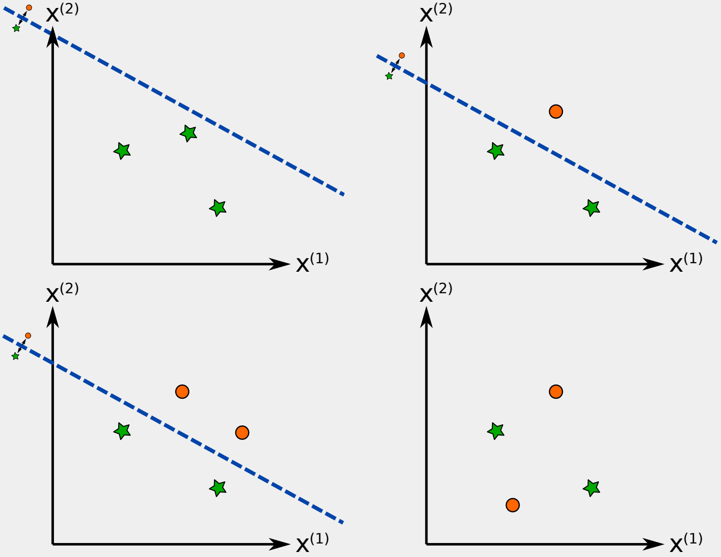
Complexity of classifiers - VC dimension

VC-Dimension (Vapnik Chervonenkis)

Let $\mathbb{F}_p$ be a set of classifiers on an n-dimensional input space. The VC-dimension $\mathrm{VC}(\mathbb{F}_p)$ 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 $\mathbb{R}^p$: $\mathrm{VC} = p + 1$
  - SVM with RBF kernel: $\mathrm{VC} = \infty$
  - Neural network with n_e edges, n_v nodes and sigmoid activation function: $\Omega(n_e^2) < \mathrm{VC} < \mathcal{O}(n_e^2 n_v^2)$ [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

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

where

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

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

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

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

Measures of model complexity - DF

- Degrees of freedom for the OLS estimate:

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

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

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

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

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

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 samples[2]
- Traditional statistics: Combine measure of accuracy (in-sample-error) with a penalty for complexity

[2] Heavy 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):

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

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]

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

- 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

- 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

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

  where $X \in \mathbb{R}^{n \times p}$ 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 $(X, \mathbf{Y}_t)$, then [Efron, 1986]

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

Model selection approaches - DF

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

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

- 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

$$\mathrm{pr}(m_i \mid x) = \frac{\mathrm{pr}(x \mid m_i)\mathrm{pr}(m_i)}{\sum_j \mathrm{pr}(x \mid m_j)\mathrm{pr}(m_j)} = \frac{\mathrm{pr}(x \mid m_i)\mathrm{pr}(m_i)}{\mathrm{pr}(x)}$$

- We compare two models m_i and m_j using

$$\frac{\mathrm{pr}(m_i \mid x)}{\mathrm{pr}(m_j \mid x)} = \frac{\frac{\mathrm{pr}(x \mid m_i)\mathrm{pr}(m_i)}{\mathrm{pr}(x)}}{\frac{\mathrm{pr}(x \mid m_j)\mathrm{pr}(m_j)}{\mathrm{pr}(x)}} = \frac{\mathrm{pr}(x \mid m_i)\mathrm{pr}(m_i)}{\mathrm{pr}(x \mid m_j)\mathrm{pr}(m_j)}$$

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

Model selection approaches - Bayes factor

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

$$\frac{\mathrm{pr}(x \mid m_i)}{\mathrm{pr}(x \mid m_j)}$$

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

$$\mathrm{pr}(x \mid m) = \int_\theta \mathrm{pr}(x \mid \theta, m)\mathrm{pr}(\theta \mid m)\mathrm{d}\theta$$

  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

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

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

where $\hat{\theta}$ refers to the maximum likeklihood 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

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

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]:

$$\mathrm{pr}(x \mid m) \approx \exp\{-\mathrm{FIA}(x; m)\}$$

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

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

  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

$$\begin{aligned} \omega(\theta) &= -\log \mathrm{pr}_\theta(y) \quad \text{(maximum likelihood), or} \\ \omega(\theta) &= \|y - X\theta\|_2^2 \quad \text{(linear regression)} \end{aligned}$$

Regularized estimate with ℓ_k-norm penalty

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

where

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

[2] Remember 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 Lagriangian

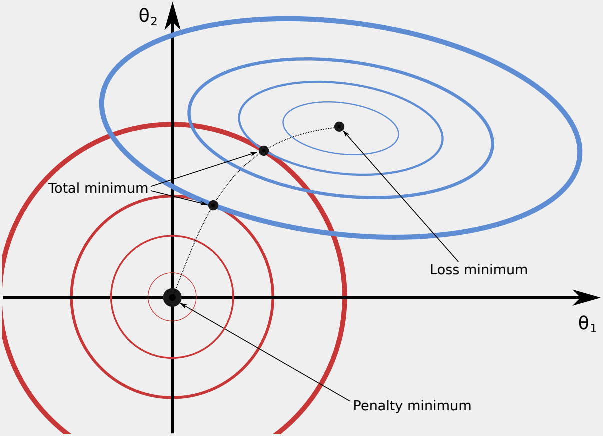
$$\hat{\theta}(\lambda) = \arg\min_{\theta} \omega(\theta) + \lambda \|\theta\|_k^k$$

At the optimum we must have

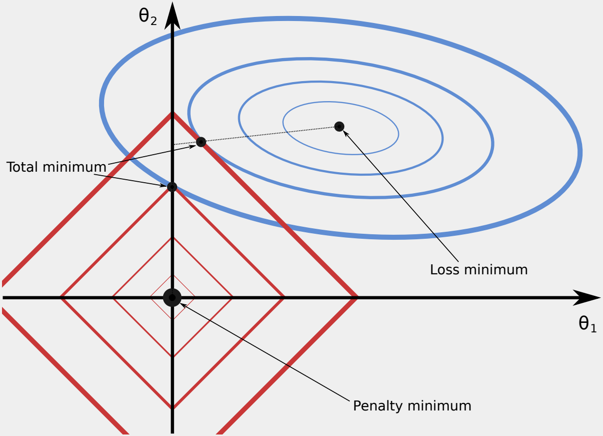
$$\nabla_\theta \, \omega(\theta) + \lambda \nabla_\theta \|\theta\|_k^k = 0$$

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

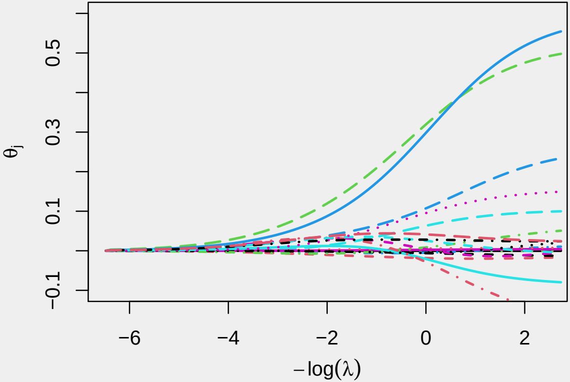
Regularization - k=2



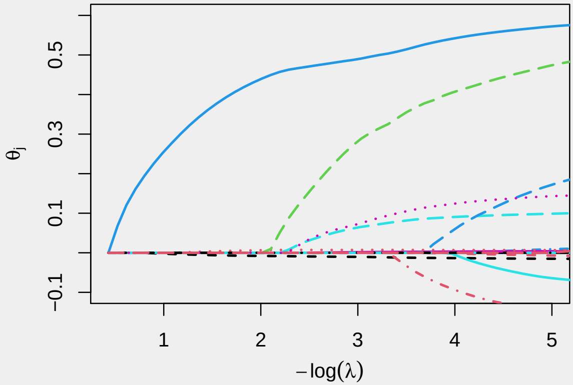
Regularization - k=1



Regularization paths - K=2

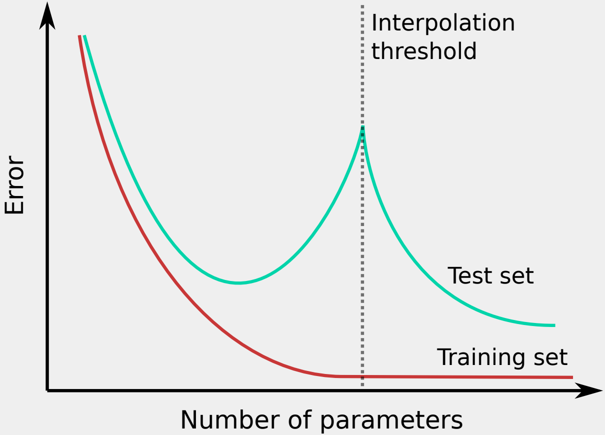


Regularization paths - k=1

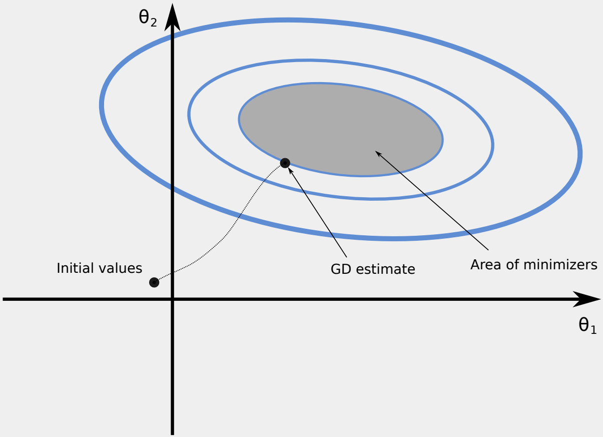


Implicit Regularization and Double Descent

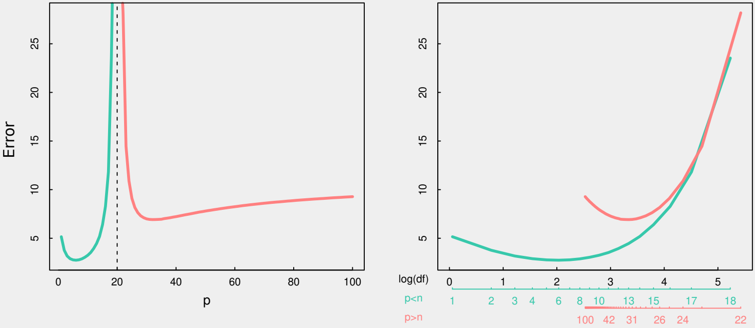
Implicit Regularization - Double descent



Implicit Regularization - Double descent



Minimum ℓ_2-norm estimate - DF



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

Implicit regularization

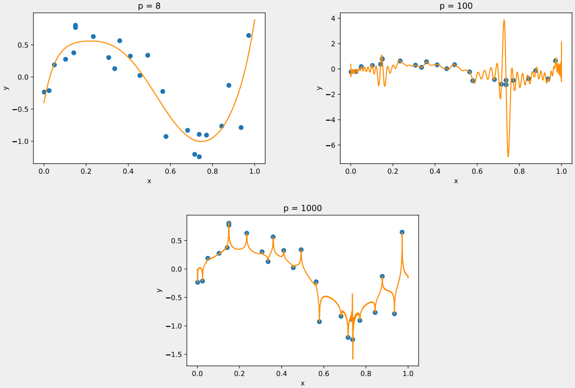


Figure: Fitting degree $d = p - 1$ Legendre polynomials. For $p > n$ the solution with the smallest ℓ_2-norm is used.

[2] Legendre 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 correspont 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 Jojic, 2016, Luan et al., 2021]
- Implicit regularization and double descent
  [Hastie et al., 2022, Luan et al., 2021, Derezinski et al., 2020, Kobak et al., 2020]

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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