Selecting g: Problem and Remedy

What is overfitting?

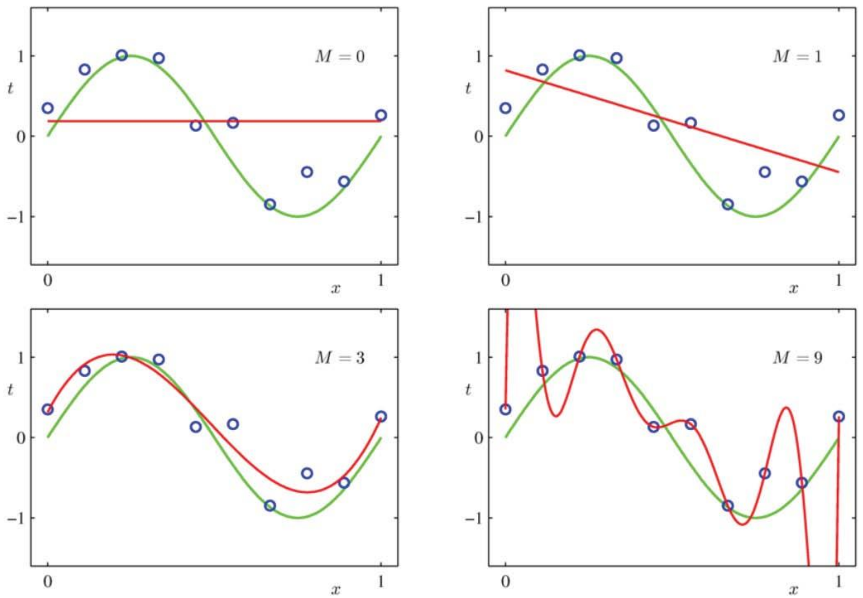
- Overfitting means low error in training and high error in test

- Overfitting is the main source of error in M.L. applications

- Usually appears when our model explains the training data too well.

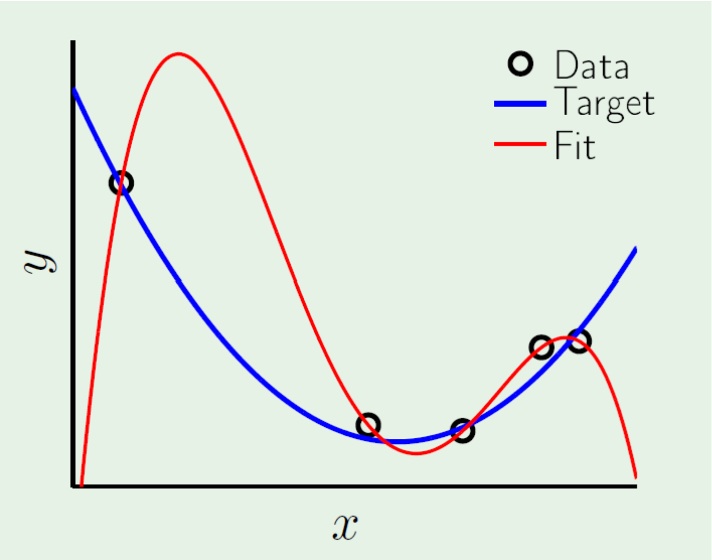
- In general is not easy to detect overfitting since depend of unknow entities (data noise)

- Most of the time overfitting is the consequence of considering a set of function $\mathcal{H}$ more complex than required……but not always !



Overfitting

Simple one-dimensional regression example with 5 data plus some noise



- In blue we show the true function generating the data, 2nd order polynomial
- In red we show the fitted function with zero in-sample-error. A 4th-order polynomial
- The sample have been overfitted !!
- Little noise in the data has mislead the learning

- The fit has zero in-sample-error but huge out-of-sample-error
- In the Bias-Variance treadoff we get BIAS=0 (in sample) but the price is to increase the VARIANCE very much.
  - $\mathbb{E}_D\left[E_{out}\left(g^{(\mathcal{D})}\right)\right] = \sigma^2 + \mathbf{bias} + \mathbf{variance}$ (for noisy signals)

Overfitting

- Why this happen?

1. STOCHASTIC ERROR : Noisy labeling, hence more complex functions are needed to get better in-sample-error

2. DETERMINISTIC NOISE : Noise from model. The complexity of the true function is not well represented by the data sample

How to protect against overfitting?

- PROBLEM: How to decide the right complexity of the solution ?
  - The noise adds independent information to the sample data
  - The ERM/SRM criteria is responsible of the final selection

- SOLUTION-1: A hard-way is to restrict the size of the $\mathcal{H}$ set. (ERM)
  - We restrict the capacity of $\mathcal{H}$ to fit noise.
  - BUT, we also restrict the capacity to find the right solution.
  - The restriction to a particular set of functions $\mathcal{H}$ is called " inductive bias"

- SOLUTION-2: A softer way is to impose additional conditions on the error function
  - We get a compromise between the best fitting function and its complexity
  - It is soft since the compromise is fixed by a weigthing parameter
  - This technique is called "regularization"

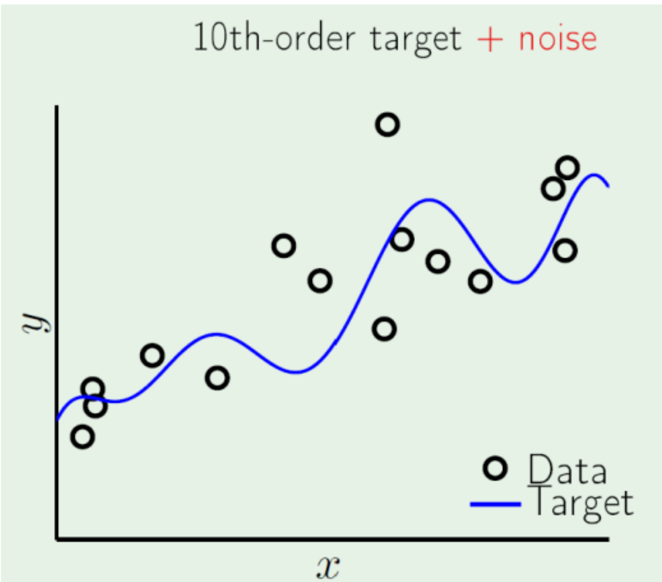
Both approaches INDUCTIVE BIAS / REGULARIZATION can be seen as using some kind of prior knowledge

QUESTION: is INDUCTIVE BIAS / REGULARIZATION necessary for the success of learning ?

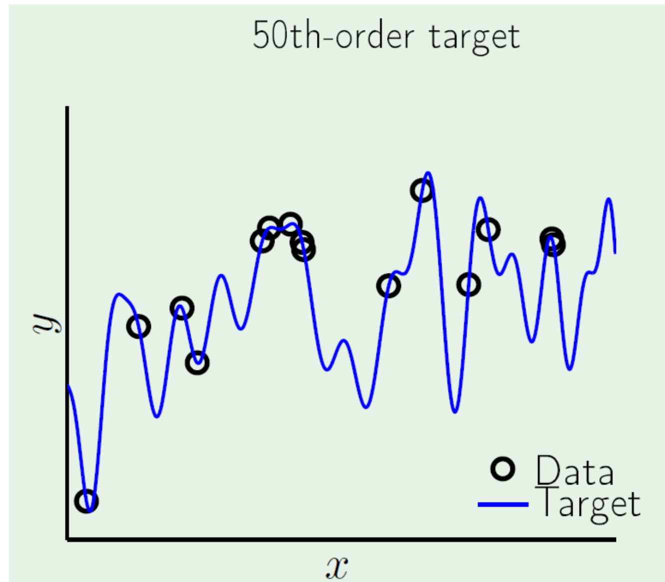
A case study

- Let consider two regression problems (*f* function).
- In both cases we have 15 polynomial data from 10th and 50th order respectively

With added noise

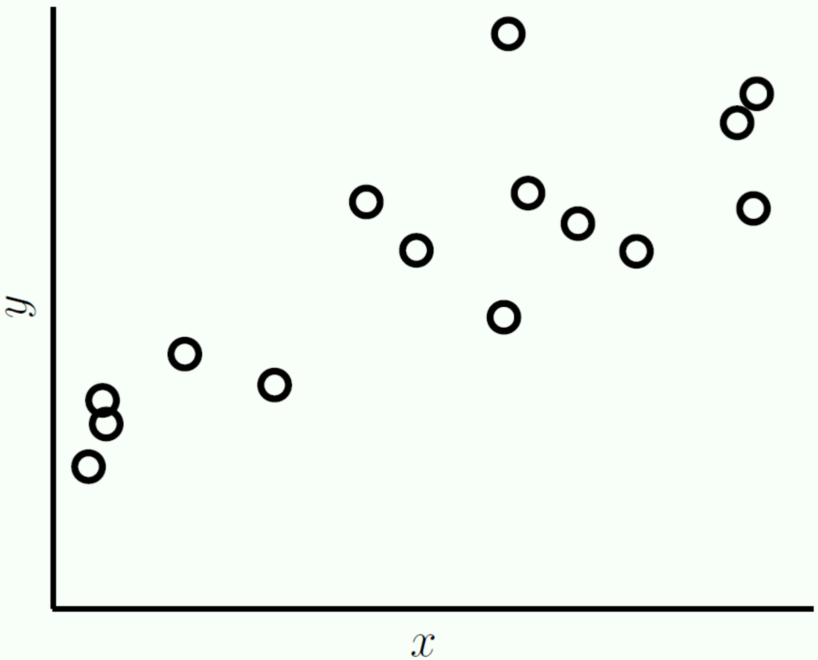


Noiseless

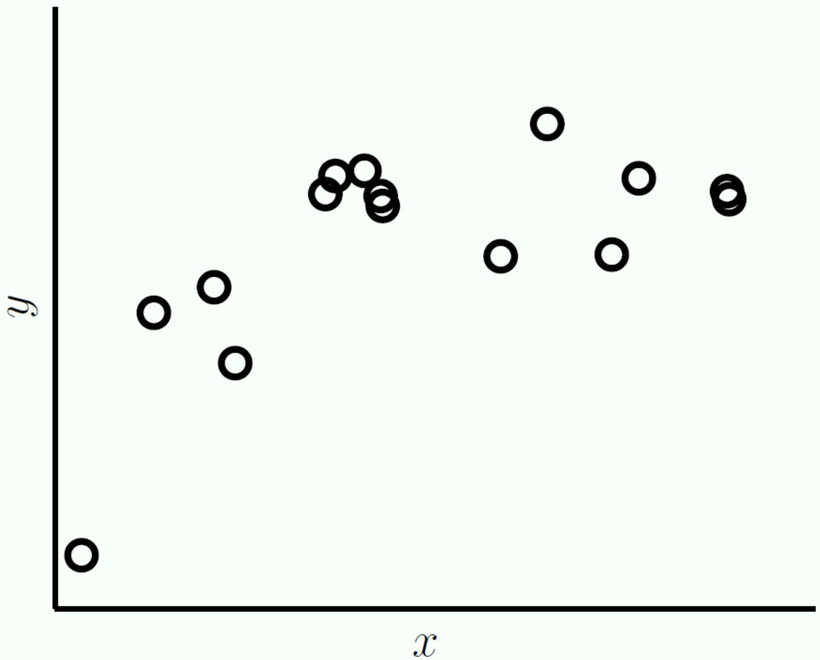


- Let's fit in both cases two polynomial: low and high order (2nd and 10th)
- Let analyze which of both produce lower out-of-sample error

Can the noise be distinguished?



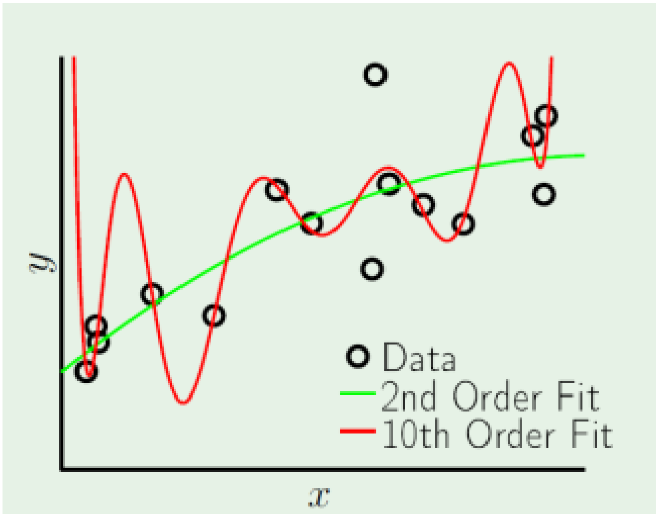
Simple f with noise.



Complex f with no noise.

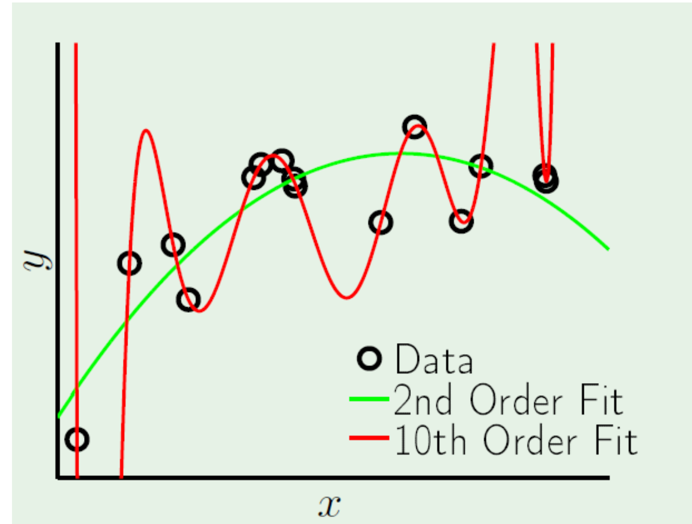
- The learning model should match the quality and quantity of the data NOT f

How are the fittings ?



Noisy low-order target

	2nd Order	10th Order
E_{in}	0.050	0.034
E_{out}	0.127	9.00

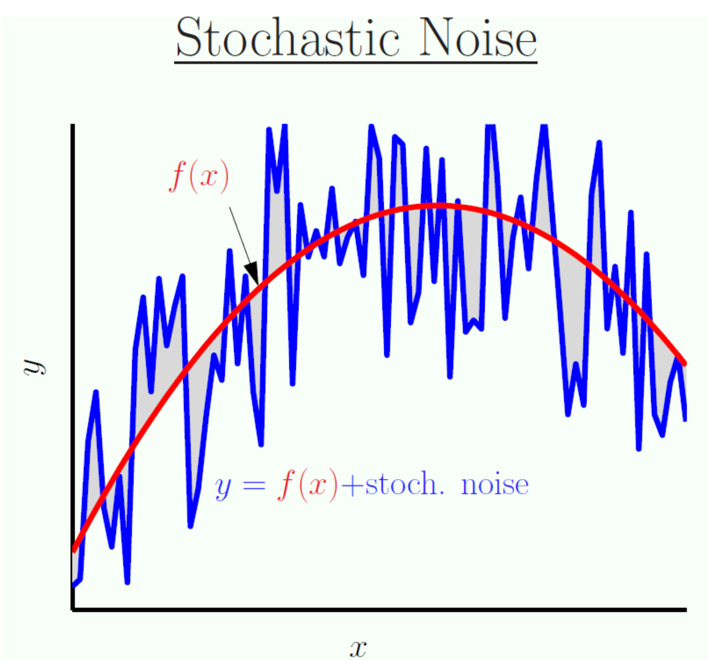


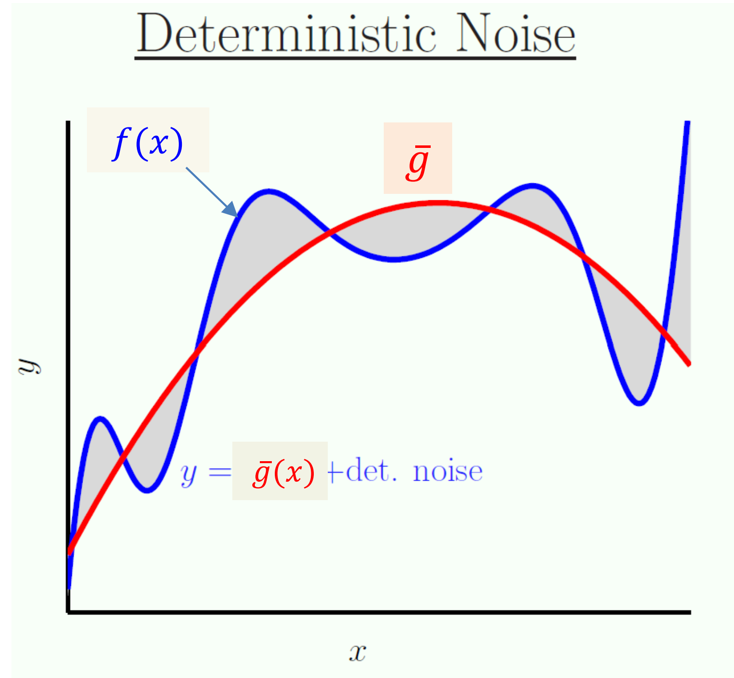
Noiseless high-order target

	2nd Order	10th Order
E_{in}	0.029	10^{-5}
E_{out}	0.120	7680

- It can be observed the smaller order polynomial presents higher in-sample error but smaller out-of sample error in both cases.
- On the left the reason is the stochastic noise, and on the right the reason is the deterministic noise.

Noise: what we cannot model





Stochastic noise: i.i.d random noise added to each data

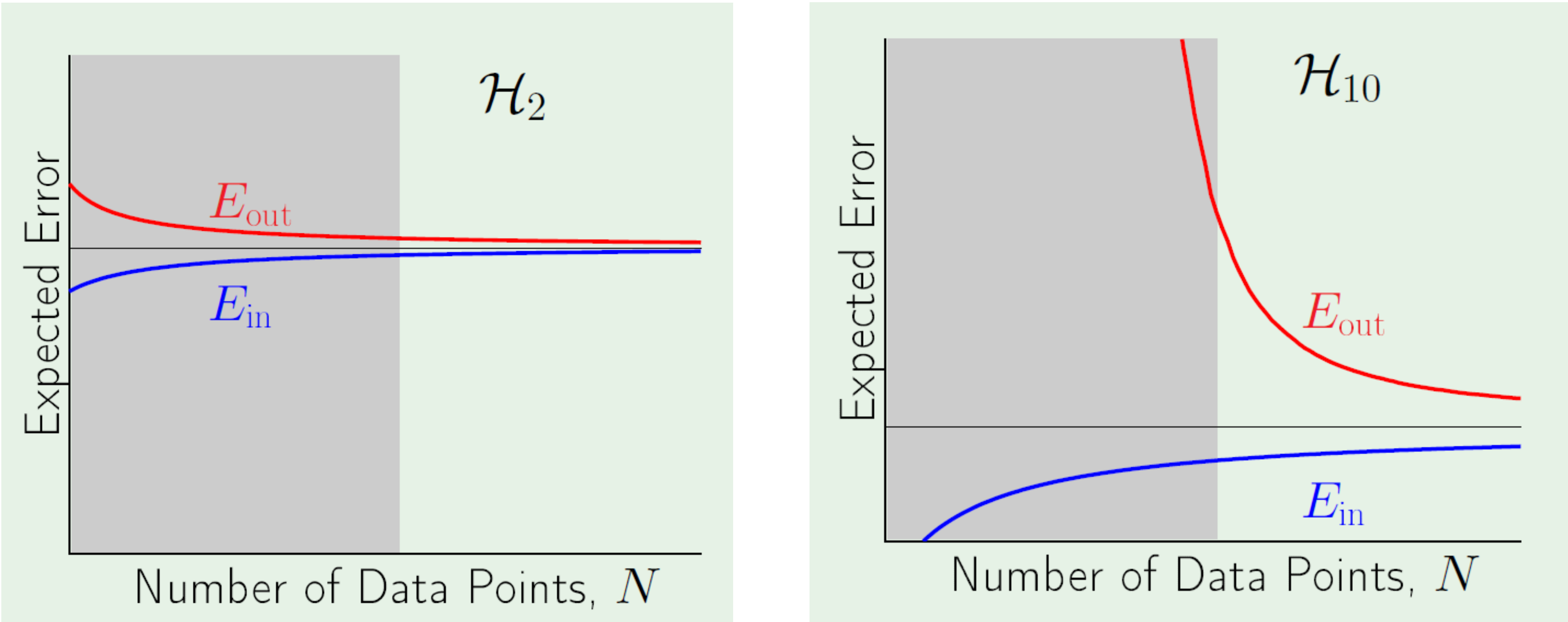
Deterministic noise: The part of the target function outside of the best fit $\bar{g}$

$$y = g^*_{\mathcal{D}}(x) + \text{noise} \qquad \text{noise} = \text{stoch. noise} + \text{det. noise}(\mathcal{H})$$

With a given data set $\mathcal{D}$ and $\mathcal{H}$ fixed , we can't differentiate between both types of noise

$$\mathbb{E}_{\mathcal{D}}\left[E_{out}\left(g^{(\mathcal{D})}\right)\right] = \sigma^2 + \text{bias} + \text{var} = \text{stoch.noise} + \text{det.noise} + \text{var}$$

Learning curves: overfitting



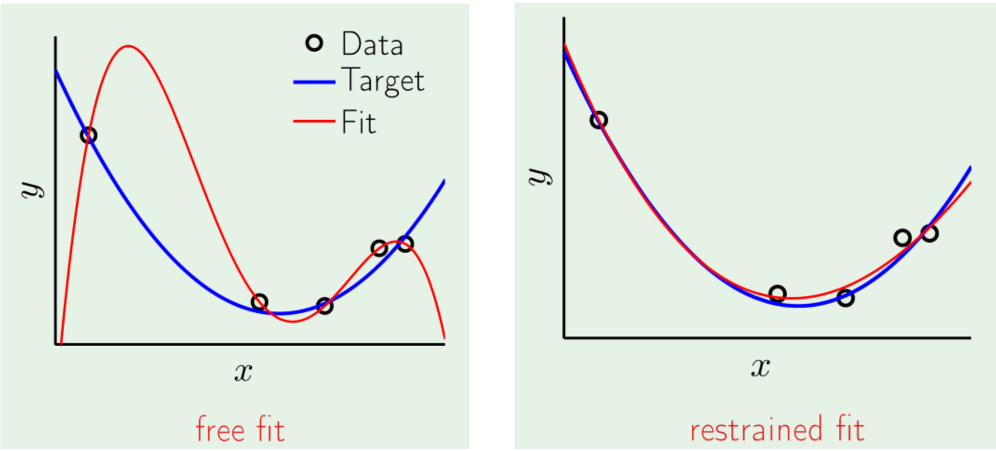
- The gray area show the range of N values, where $\mathcal{H}_{10}$ has lower E_{in} and higher E_{out}: overfitting is present.
- The learning curves show typical behaviour of a simple and a complex model respectively.
- These pictures show the importance of the data size in the overfitting

- **WHAT MATTERS IS HOW THE MODEL COMPLEXITY MATCHES THE QUALITY AND QUANTITY OF DATA WE HAVE**

REGULARIZATION: An smart mechanism to prevent overfitting

Regularization

- Idea: Constraint the learning model to improve the out-of-sample error



The figures show the dramatic improvement in the fit with a small amount of regularization

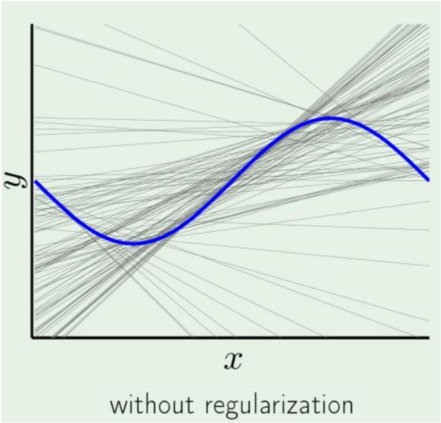
- Regularization is an heuristic approach although is in close connection with the optimization techniques

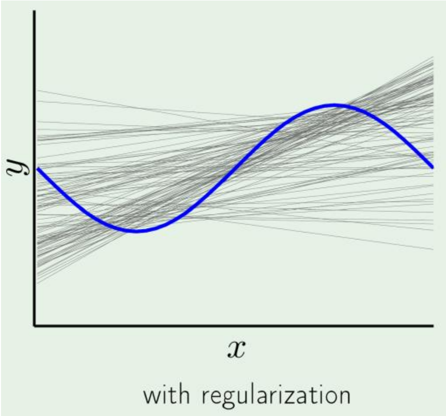
- According to the Approx.-Genera. tradeoff $E_{out}(g) \leq E_{in}(g) + \Omega(\mathcal{H})$, regularization minimizes the right hand of the inequality not only the in-sample error

- According to the Bias-Variance tradeoff, regularization increases lightly the Bias to strongly decrease the Variance

Constraining the model helps

- The **weight decay** technique measures the complexity of a hypothesis h by the size of the coefficients used to represent h.



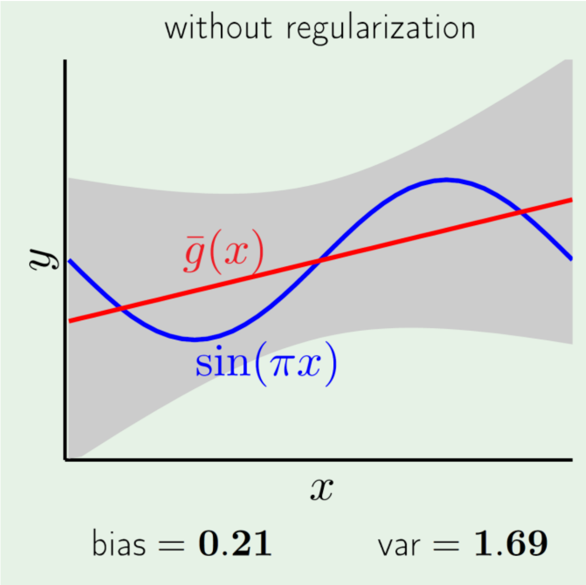


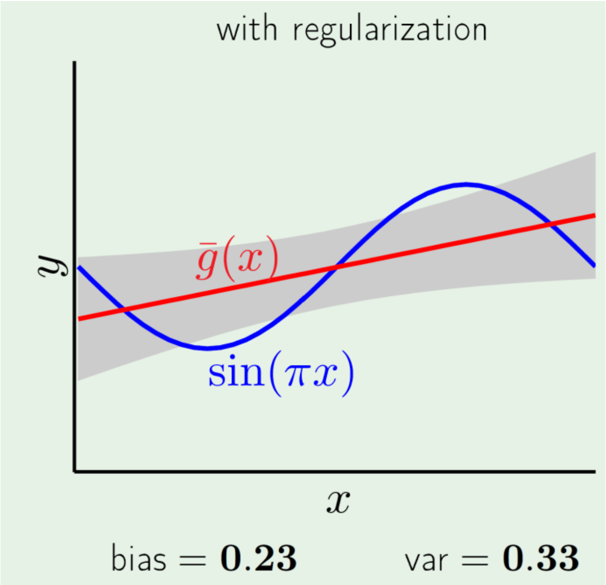
- The figure shows the result of applying weight decay to fit the target $f(x)=\sin(\pi x)$, $x\in[-1,1]$, using samples of N=2 (lines) , x is sampled uniformly in [-1,1]

- Without regularization shows a very high variability in the learning function depending on the sample x

- With regularization (constraining weights to be small) shows how the set of learning functions is much more stable

Constraining the model helps !





- Let analyze the learning **using the Bias-Variace tradeoff**

- Without regularization we observe a l**ower bias** and **higher variance**
- With regularization we observe one **light increased bias** and a **large decrease in variance**
- In total the regularization provides a learned function with smaller out-of-sample error
- **Regularization: we sacrifice a little** bias **for a significant gain in** var

Regularization: Some theory

- **General linear regression problem** : The goal is minimize the in-sample squared error

$$E_{in}(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}(\mathbf{w}^T\mathbf{z}_n - y_n)^2$$

over the hypothesis in $\mathcal{H}_Q$ in order to get $\mathbf{w}_{lin} = \underset{\mathbf{w}}{\operatorname{argmin}}\, E_{in}(\mathbf{w})$

How to restrict the values of the vector $\mathbf{w}_{lin}$ in order to get a better Bias-Variance tradeoff?

- Hard constraints: imposes that some weights must be zero

$$H_2 = \{h \in H_{10} |\, w_k = 0, k > 2\}$$

- Soft constraints: imposes that some positive function of the weights be bounded:

$$\sum_{i=0}^{Q} w_i^2 \leq C$$

Regularization: Examples

Examples: (1) $\sum_{q=0}^{Q} w_q^2 \leq C$, (2) $\sum_{q=0}^{Q} |w_q| \leq C$, (3) $\left(\sum_{q=0}^{Q} w_q\right)^2 \leq C$, (4) $\sum_{q=0}^{Q} \gamma_q w_q^2 \leq C$

- In (1), solutions with low values, but not necessarily zero are encouraged
- In (2), we encourage some values to be zero (LASSO, good for feature selection !)
- In (3), we encourage the same contribution of positive and negative weigths
- In (4), according to the coefficients we encourage the contribution of the weights

- Each restriction encourages a specific solution and defines an optimization problem that must be solved

Regularization: solving the problem

- The in-sample optimization problem becomes

$$\min_{\mathbf{w}} E_{in}(\mathbf{w}) \quad \text{subject to } \mathbf{w}^T\mathbf{w} \leq C$$

the learning algorithm chooses the best solution given the total budget *C.*

- Let $\mathrm{H}(C) = \{h \mid h(\boldsymbol{z}) = \mathbf{w}^{\mathrm{T}}\mathbf{z},\ \mathbf{w}^{\mathrm{T}}\mathbf{w} \leq C\}$, the new class of functions. Clearly the *C* value defines a constraint on the class of hypothesis.

- Let's define $w_{reg} = \arg\min E_{in}(\mathbf{w}) \quad \text{subject to } \mathbf{w}^T\mathbf{w} \leq C$

- If $\boldsymbol{w}_{lin} \in \mathrm{H}(C)$ then $\boldsymbol{w}_{reg} = \boldsymbol{w}_{lin}$, and $\boldsymbol{w}_{reg}^T\boldsymbol{w}_{reg} \leq C$ and the constraint is redundant. But if $\boldsymbol{w}_{lin} \notin \mathrm{H}(C)$ this means $\boldsymbol{w}_{lin}^T\boldsymbol{w}_{lin} > C$ and in this case the best $\boldsymbol{w}_{reg} \in \mathrm{H}$ belong to $\boldsymbol{w}_{reg}^T\boldsymbol{w}_{reg} = C$

- Both cases can be considered solving for

$$w_{reg} = \arg\min E_{in}(\mathbf{w}) \quad \text{subject to } \mathbf{w}^T\mathbf{w} = C$$

Lagrange Multipliers

- We want to convert our constrained minimization problem in an unconstraint minization

$$\min_{\mathbf{w}} E_{in}(\mathbf{w}) \quad \text{subject to } \mathbf{w}^T\mathbf{w} = C \quad \Rightarrow \quad \min_{\mathbf{w}} E_{in}(\mathbf{w}) + \lambda_C \, \mathbf{w}^T\mathbf{w}, \quad \lambda_C > 0$$

Using Lagrange Multipliers

$$\boldsymbol{w}_{reg} = \arg\min_{w,\beta} E_{in}(\mathbf{w}) - \beta(\mathbf{w}^T\mathbf{w} - C)$$

- β is a Lagrange Multiplier which value shows us the strength imposed on the constraint in order to get the optimum. (What β values are expected when $\boldsymbol{w}_{lin} \in \mathrm{H}(C)$ or $\boldsymbol{w}_{lin} \notin \mathrm{H}(C)$?)

The Lagrangian can be rewritten as an expression with only one free parameter λ_C

$$\mathbf{w}_{reg} = \underset{\mathbf{w}}{\operatorname{argmin}} E_{reg}(\boldsymbol{w}) = \underset{\mathbf{w}}{\operatorname{argmin}} (E_{in}(\mathbf{w}) + \lambda_C \, \mathbf{w}^T\mathbf{w})$$

- Let's define the augmented error for each hypotesis $\mathbf{w}$:

$$E_{aug}(\mathbf{w}, \lambda, \Omega) = E_{in}(\mathbf{w}) + \frac{\lambda}{N}\Omega(\mathbf{w})$$

- The λ parameter defines the intensity of the regularization
- $\Omega(\mathbf{w}) = \mathbf{w}^T\mathbf{w}$ defines a complexity measure for each hipothesis

Regularized linear model: Weight Decay

- Using matrix notation we have: $E_{aug}(\mathbf{w}) = \|Z\mathbf{w} - \boldsymbol{y}\|^2 + \lambda\|\mathbf{w}\|^2$

- $\mathbf{w}_{reg}$ is the solution of the equation $\nabla_{\mathbf{w}} E_{aug}(\mathbf{w})$ = $\nabla_{\mathbf{w}} \left(E_{in}(\mathbf{w}) + \lambda \mathbf{w}\mathbf{w}^T\right) = 0$

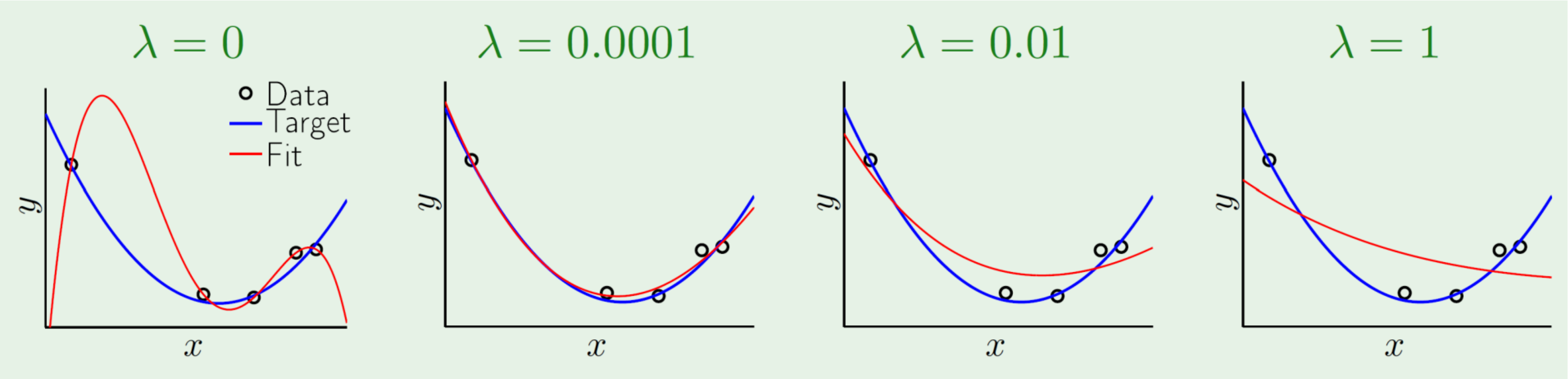
$$\nabla_{\mathbf{w}} E_{aug} = 2\mathrm{Z}^T(\mathrm{Z}\mathbf{w} - \boldsymbol{y}) + \lambda\mathbf{w}^T = 0 \quad \Rightarrow \quad \mathbf{w}_{reg} = (\mathrm{Z}^{\mathrm{T}}\mathrm{Z} + \lambda\mathrm{I})^{-1}\mathrm{Z}^{\mathrm{T}}\boldsymbol{y}$$

- As expected $\mathbf{w}_{reg} \to 0$ when $\lambda \to \infty$
- The predictions on the in-sample data are given by: $\hat{\boldsymbol{y}} = Z\mathbf{w}_{reg} = H(\lambda)\boldsymbol{y}$

$$\mathrm{H}(\lambda) = \mathrm{Z}\left(\mathrm{Z}^{\mathrm{T}}\mathrm{Z} + \lambda\mathrm{I}\right)^{-1}\mathrm{Z}^{\mathrm{T}}$$

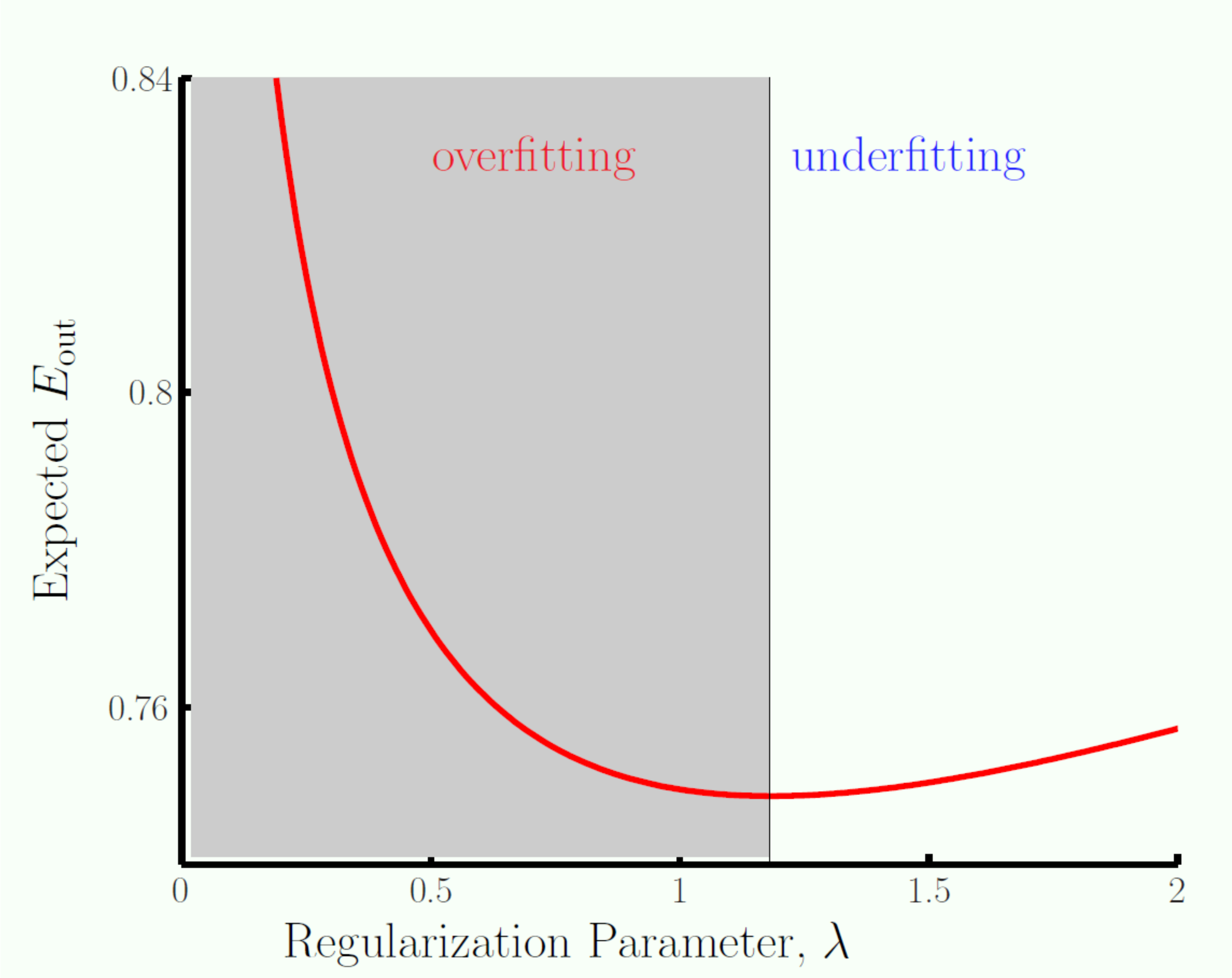
- The matrix hat $\mathrm{H}(\lambda)$ plays a relevant role in defining the efective complexity of the model
  - λ=0, H is the hat-matrix of the linear regression
  - The vector of in-sample errors is : $\boldsymbol{y} - \hat{\boldsymbol{y}} = \left(\mathrm{I} - H(\lambda)\right)\boldsymbol{y}$
  - The in-sample error is : $E_{in}\left(\mathbf{w}_{reg}\right) = \frac{1}{N}\boldsymbol{y}^T(\mathrm{I} - H(\lambda))^2\boldsymbol{y}$

Regularization: Linear models + w.d.



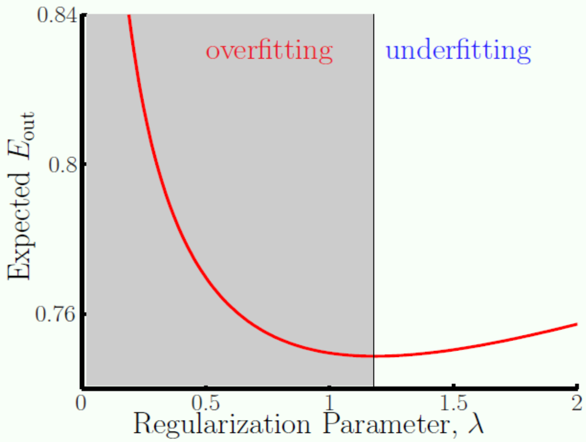
- The figure shows the result of applying different amount of regularization to the same example using weight decay
- It can be seen that non-regularization or too much regularization increases the adjustment error. In the first case due to the variance in the second case due to the bias.

Overfitting & Underfitting



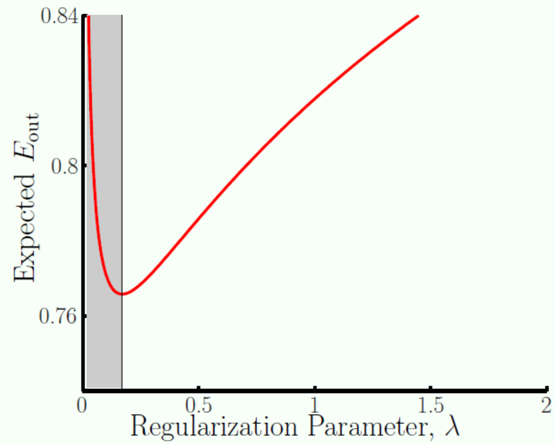
Variations on Weight Decay

Uniform Weight Decay



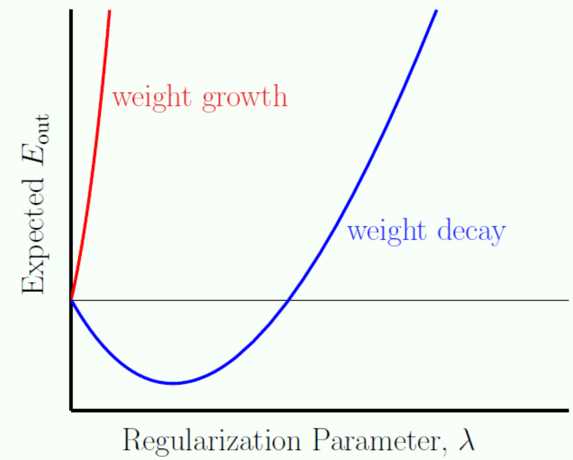
$$\sum_{q=0}^{Q} w_q^2$$

Low Order Fit



$$\sum_{q=0}^{Q} q w_q^2$$

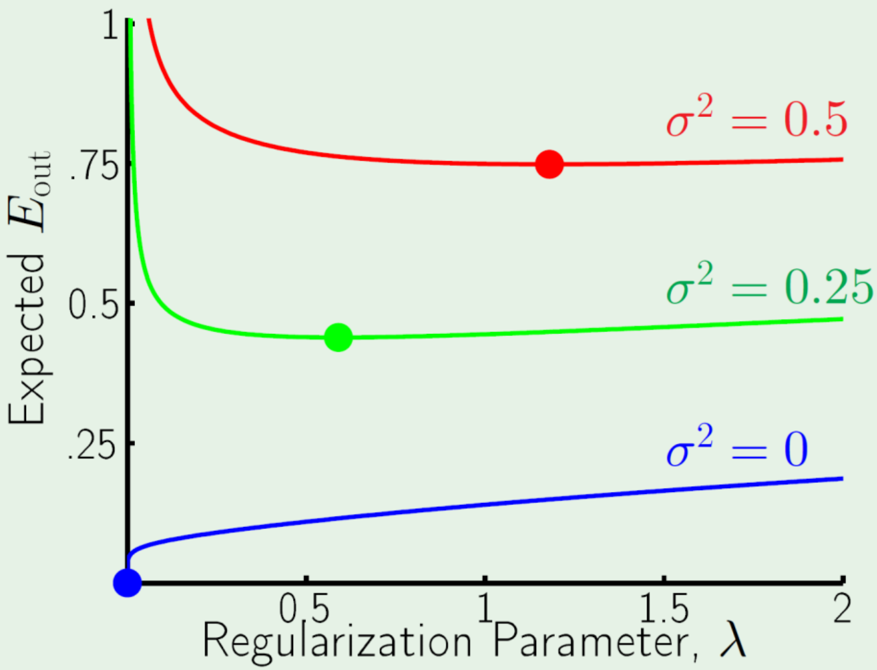
Weight Growth!



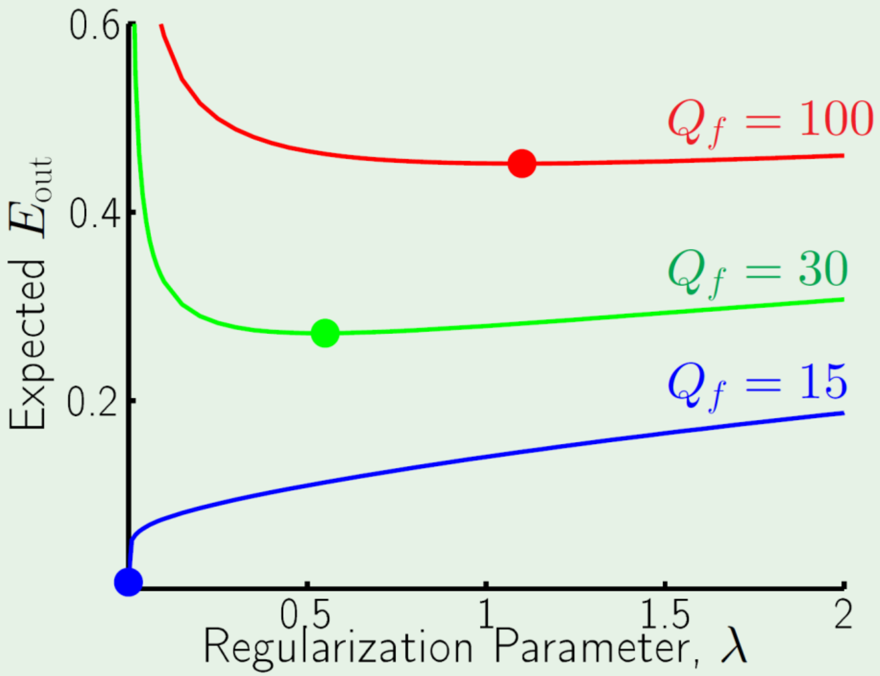
$$\sum_{q=0}^{Q} \frac{1}{w_q^2}$$

$\mathbf{w}^T \Gamma^T \Gamma \mathbf{w} \le \boldsymbol{C}$ Tikhonov Regularizer

Example of Regularization and noise



Stochastic noise



Deterministic noise

$f \in \mathcal{K}(pol. order\ 15)$

Uniform regularizer: $\Omega(\mathbf{w}) = \sum_{q=0}^{15} w_q^2$

Choosing a Regularized: A Practitioner's Guide….

- Leasson learned: Some form of regularization is necessary

- The perfect regularizer: does not exist
  - constrain in the 'direction' of the target function.
  - target function is **unknown** (going around in circles).

- The guiding principle:
  - constrain in the 'direction' of smoother (usually simpler) hypotheses
  - hurts your ability to fit the 'high frequency' noise
  - smoother and simpler usually means –→ weight decay not weight growth.

- What if you choose the wrong regularizer?
  - You still have λ to play with — **validation.**

How Does Regularization Work?

- Stochastic noise –→ nothing you can do about that.
- Good features –→ helps to reduce deterministic noise.
- Regularization:
  – Helps to combat what noise remains, especially when N is small.
  – Typical modus operandi: sacrifice a little **bias** for a huge improvement in **var**.
  – VC angle: you are using a smaller $\mathcal{H}$ without sacrificing too much E_{in}