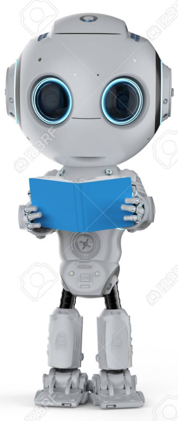
Machine Learning CS60050

Computational Learning Theory

(Regularization)



Learning From Data

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Lecture 12: Regularization

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Outline

- Regularization - informal
- Regularization - formal
- Weight decay
- Choosing a regularizer

Two approaches to regularization

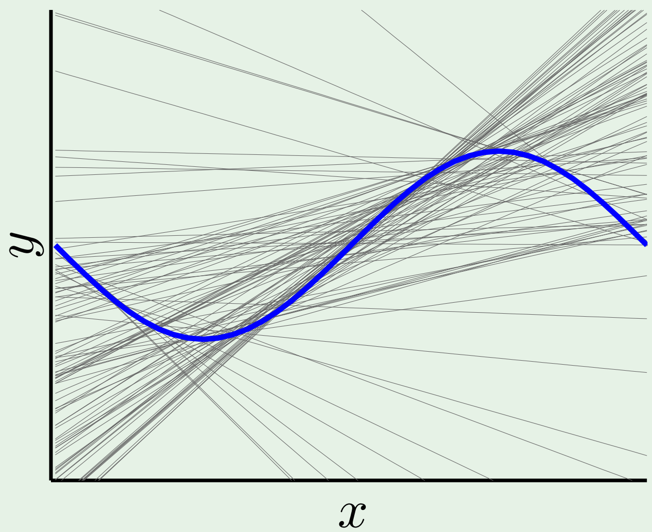
Mathematical:

Ill-posed problems in function approximation

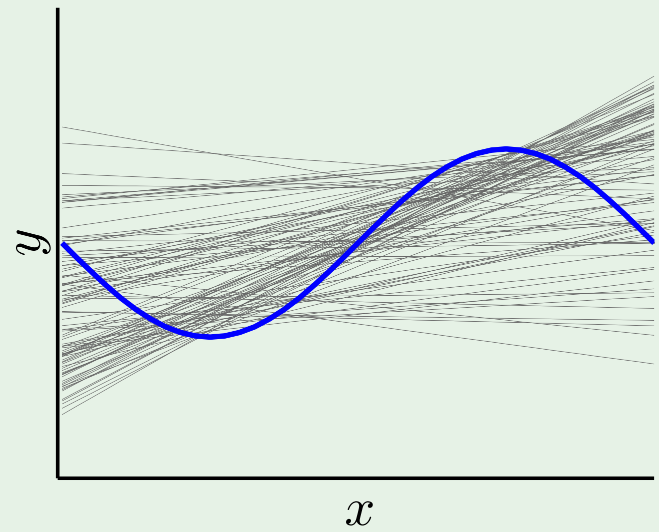
Heuristic:

Handicapping the minimization of E_{in}

A familiar example



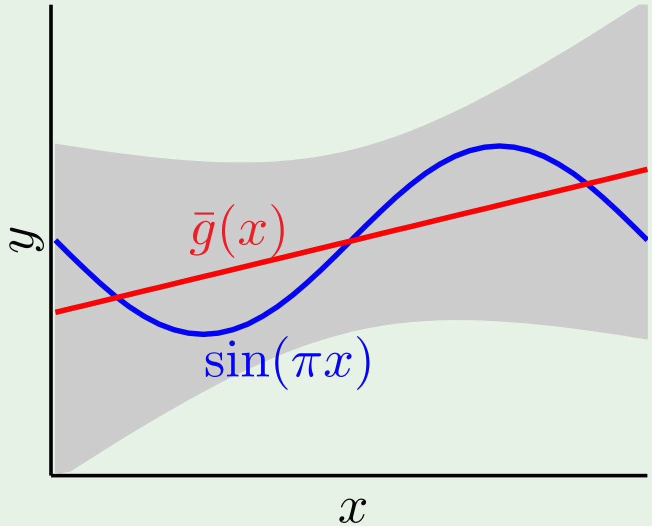
without regularization



with regularization

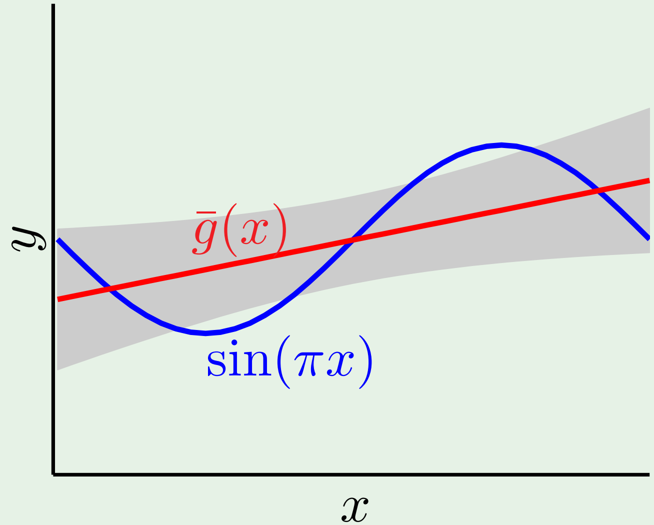
and the winner is . . .

without regularization



bias $=$ **0.21** var $=$ **1.69**

with regularization



bias $=$ **0.23** var $=$ **0.33**

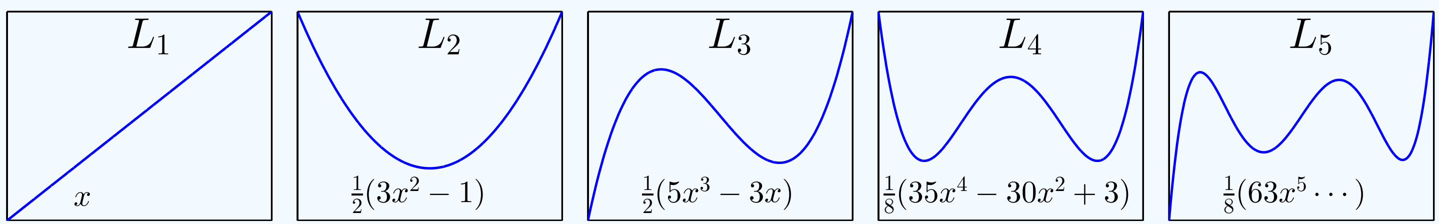
The polynomial model

$\mathcal{H}_Q$: polynomials of order Q

linear regression in $\mathcal{Z}$ space

$$\mathbf{z} = \begin{bmatrix} 1 \\ L_1(x) \\ \vdots \\ L_Q(x) \end{bmatrix} \qquad \mathcal{H}_Q = \left\{ \sum_{q=0}^{Q} w_q \, L_q(x) \right\}$$

Legendre polynomials:



Unconstrained solution

Given $(x_1, y_1), \cdots, (x_N, y_n) \quad \longrightarrow \quad (\mathbf{z}_1, y_1), \cdots, (\mathbf{z}_N, y_n)$

Minimize $E_{\text{in}}(\mathbf{w}) = \dfrac{1}{N} \displaystyle\sum_{n=1}^{N} (\mathbf{w}^{\mathsf{T}} \mathbf{z}_n - y_n)^2$

Minimize $\frac{1}{N} (\mathrm{Z}\mathbf{w} - \mathbf{y})^{\mathsf{T}} (\mathrm{Z}\mathbf{w} - \mathbf{y})$

$$\mathbf{w}_{\text{lin}} = (\mathrm{Z}^{\mathsf{T}}\mathrm{Z})^{-1}\mathrm{Z}^{\mathsf{T}}\mathbf{y}$$

Constraining the weights

Hard constraint: $\mathcal{H}_2$ is constrained version of $\mathcal{H}_{10}$ with $w_q = 0$ for $q > 2$

Softer version: $\displaystyle\sum_{q=0}^{Q} w_q^2 \le C$ "**soft-order**" constraint

Minimize $\frac{1}{N}(\mathrm{Z}\mathbf{w} - \mathbf{y})^{\intercal}(\mathrm{Z}\mathbf{w} - \mathbf{y})$

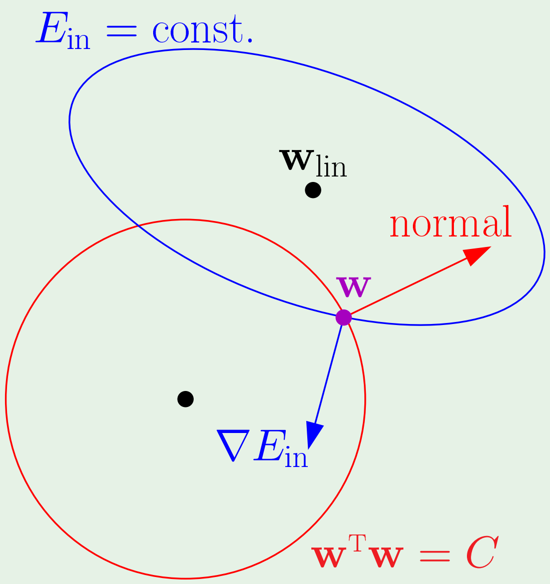
subject to: $\mathbf{w}^{\intercal}\mathbf{w} \le C$

Solution: $\mathbf{w}_{\text{reg}}$ instead of $\mathbf{w}_{\text{lin}}$

Solving for $\mathbf{w}_{\text{reg}}$

Minimize $\quad E_{\text{in}}(\mathbf{w}) \;=\; \frac{1}{N}\,(\mathrm{Z}\mathbf{w}-\mathbf{y})^{\mathsf{T}}(\mathrm{Z}\mathbf{w}-\mathbf{y})$

subject to: $\quad \mathbf{w}^{\mathsf{T}}\mathbf{w} \le C$



$$\nabla E_{\text{in}}(\mathbf{w}_{\text{reg}}) \propto \; -\mathbf{w}_{\text{reg}}$$

$$= \; -2\frac{\lambda}{N}\mathbf{w}_{\text{reg}}$$

$$\nabla E_{\text{in}}(\mathbf{w}_{\text{reg}}) + 2\frac{\lambda}{N}\mathbf{w}_{\text{reg}} \;=\; \mathbf{0}$$

Minimize $\quad E_{\text{in}}(\mathbf{w}) + \frac{\lambda}{N}\mathbf{w}^{\mathsf{T}}\mathbf{w} \qquad \boxed{C\uparrow \quad \lambda\downarrow}$

Augmented error

Minimizing $E_{\text{aug}}(\mathbf{w}) = E_{\text{in}}(\mathbf{w}) + \frac{\lambda}{N}\mathbf{w}^{\intercal}\mathbf{w}$

$= \frac{1}{N}(\mathrm{Z}\mathbf{w} - \mathbf{y})^{\intercal}(\mathrm{Z}\mathbf{w} - \mathbf{y}) + \frac{\lambda}{N}\mathbf{w}^{\intercal}\mathbf{w}$ unconditionally

– solves –

Minimizing $E_{\text{in}}(\mathbf{w}) = \frac{1}{N}(\mathrm{Z}\mathbf{w} - \mathbf{y})^{\intercal}(\mathrm{Z}\mathbf{w} - \mathbf{y})$

subject to: $\mathbf{w}^{\intercal}\mathbf{w} \leq C$ $\longleftarrow$ VC formulation

The solution

Minimize $\quad E_{\text{aug}}(\mathbf{w}) = E_{\text{in}}(\mathbf{w}) + \frac{\lambda}{N}\mathbf{w}^{\mathsf{T}}\mathbf{w}$

$$= \frac{1}{N}\left((\mathrm{Z}\mathbf{w} - \mathbf{y})^{\mathsf{T}}(\mathrm{Z}\mathbf{w} - \mathbf{y}) \;+\; \lambda\, \mathbf{w}^{\mathsf{T}}\mathbf{w}\right)$$

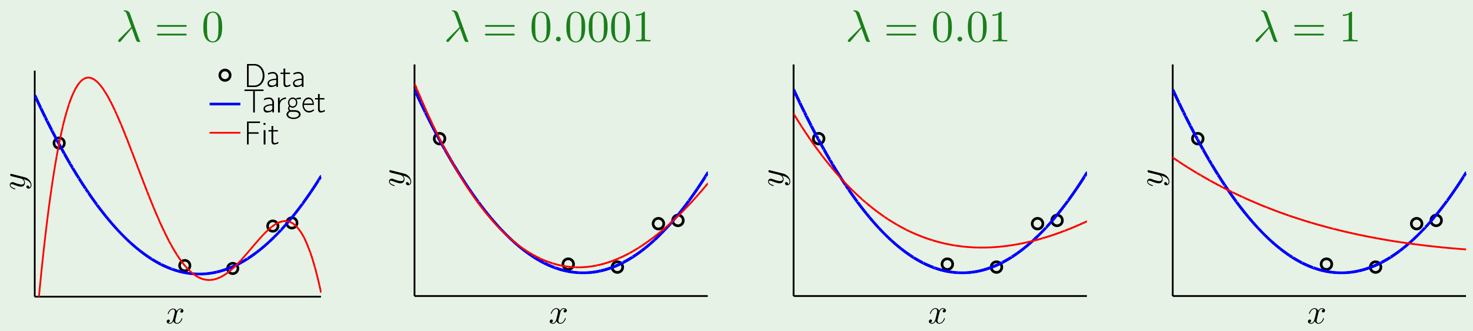
$$\nabla E_{\text{aug}}(\mathbf{w}) = \mathbf{0} \qquad \Longrightarrow \qquad \mathrm{Z}^{\mathsf{T}}(\mathrm{Z}\mathbf{w} - \mathbf{y}) + \lambda\mathbf{w} = \mathbf{0}$$

$$\boxed{\mathbf{w}_{\text{reg}} = (\mathrm{Z}^{\mathsf{T}}\mathrm{Z} + \lambda\mathrm{I})^{-1}\,\mathrm{Z}^{\mathsf{T}}\mathbf{y}}$$ (with regularization)

as opposed to $\quad \mathbf{w}_{\text{lin}} = (\mathrm{Z}^{\mathsf{T}}\mathrm{Z})^{-1}\mathrm{Z}^{\mathsf{T}}\mathbf{y}$ (without regularization)

The result

Minimizing $\quad E_{\text{in}}(\mathbf{w}) + \frac{\lambda}{N}\,\mathbf{w}^{\intercal}\mathbf{w} \quad$ for different λ's:



overfitting $\longrightarrow \quad \longrightarrow \quad \longrightarrow \quad \longrightarrow$ **underfitting**

Weight 'decay'

Minimizing $\quad E_{\text{in}}(\mathbf{w}) + \frac{\lambda}{N}\,\mathbf{w}^{\intercal}\mathbf{w} \quad$ is called weight *decay*. Why?

Gradient descent:

$$\mathbf{w}(t+1) = \mathbf{w}(t) \;-\; \eta\,\nabla E_{\text{in}}\big(\mathbf{w}(t)\big) \;-\; 2\,\eta\,\frac{\lambda}{N}\,\mathbf{w}(t)$$

$$= \mathbf{w}(t)\;(1 - 2\eta\frac{\lambda}{N}) - \eta\,\nabla E_{\text{in}}\big(\mathbf{w}(t)\big)$$

Applies in neural networks:

$$\mathbf{w}^{\intercal}\mathbf{w} = \sum_{l=1}^{L}\sum_{i=0}^{d^{(l-1)}}\sum_{j=1}^{d^{(l)}}\left(w_{ij}^{(l)}\right)^2$$

Variations of weight decay

Emphasis of certain weights: $\sum_{q=0}^{Q} \gamma_q \, w_q^2$

Examples:

$\gamma_q = 2^q \implies$ **low-order fit**

$\gamma_q = 2^{-q} \implies$ **high-order fit**

Neural networks: different layers get different γ's

Tikhonov regularizer: $\mathbf{w}^{\mathsf{T}} \Gamma^{\mathsf{T}} \Gamma \mathbf{w}$

Even weight growth!

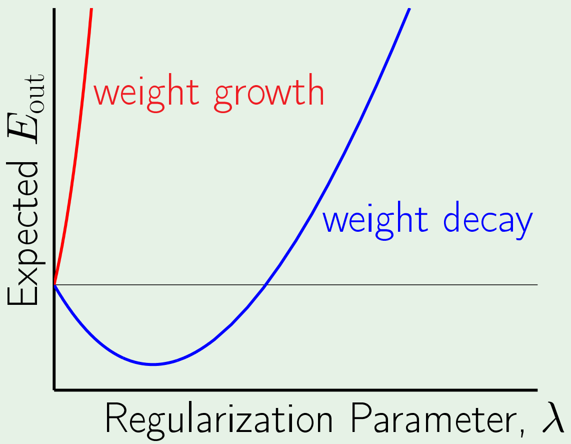
We 'constrain' the weights to be large - bad!

Practical rule:

stochastic noise is 'high-frequency'

deterministic noise is also non-smooth

$\Longrightarrow$ constrain learning towards smoother hypotheses



General form of augmented error

Calling the regularizer $\Omega \;=\; \Omega(h)$, we minimize

$$E_{\text{aug}}(h) \;= E_{\text{in}}(h) \;+\; \frac{\lambda}{N}\Omega(h)$$

Rings a bell? $\quad\downarrow\downarrow$

$$E_{\text{out}}(h) \;\leq\; E_{\text{in}}(h) \;+\; \Omega(\mathcal{H})$$

E_{aug} is better than E_{in} as a proxy for E_{out}

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- Regularization - informal
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The perfect regularizer Ω

Constraint in the ‘direction’ of the target function (going in circles ☺)

Guiding principle:

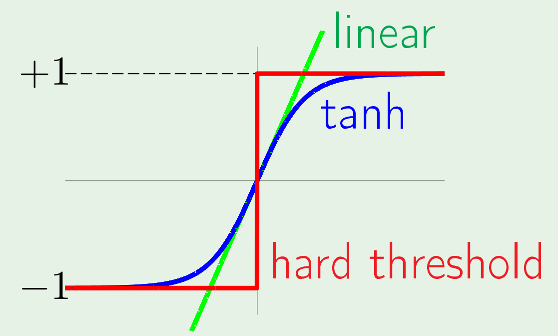
Direction of **smoother** or “simpler”

Chose a bad Ω?

We still have λ!

Neural-network regularizers

Weight decay: From linear to logical



Weight elimination:

Fewer weights $\Longrightarrow$ smaller VC dimension

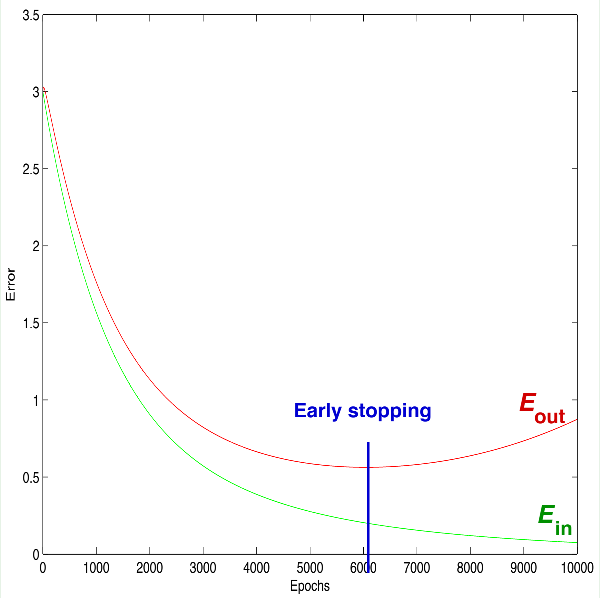
Soft weight elimination:

$$\Omega(\mathbf{w}) = \sum_{i,j,l} \frac{\left(w_{ij}^{(l)}\right)^2}{\beta^2 + \left(w_{ij}^{(l)}\right)^2}$$

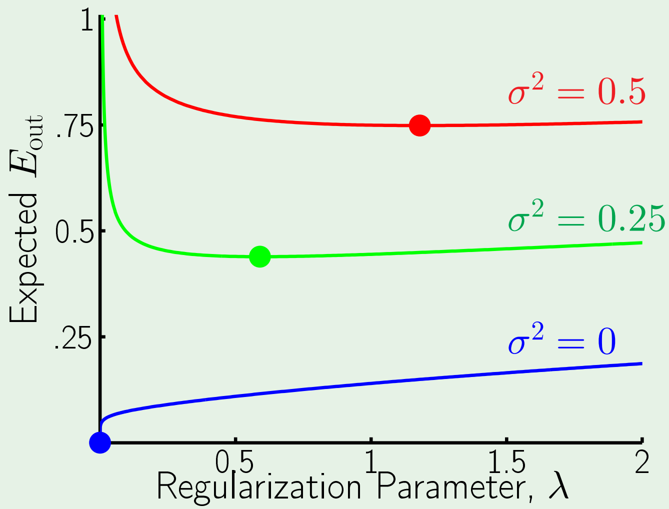
Early stopping as a regularizer

Regularization through the optimizer!

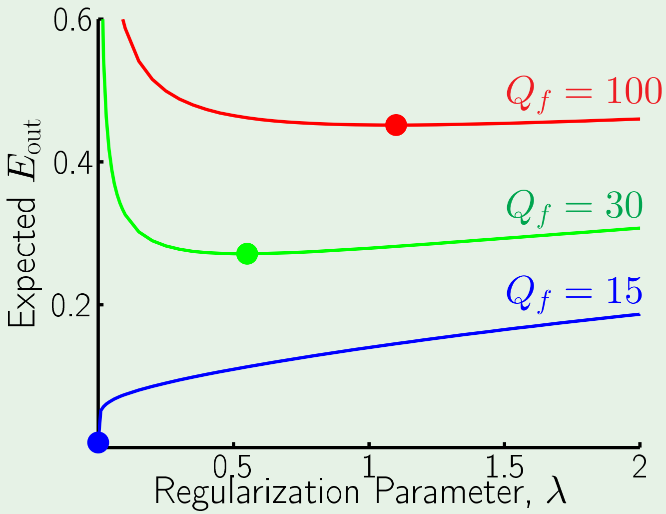
When to stop? **validation**



The optimal λ



Stochastic noise



Deterministic noise

Thank You!