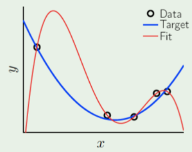
CSE4088 Introduction to Machine Learning

Regularization

Review of last lecture

- Overfitting

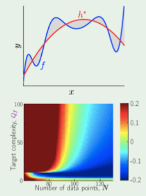
Fitting the data more than is warranted



VC allows it; doesn't predict it

Fitting the noise, stochastic/deterministic

- Deterministic noise



Outline

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

Two approaches to regularization

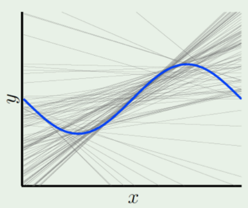
Mathematical:

Ill-posed problems in function approximation

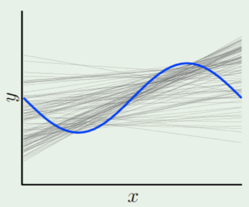
Heuristic:

Handicapping the minimization of E_{in}

A familiar example



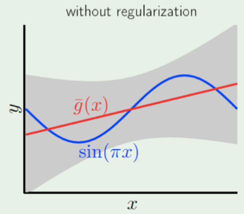
without regularization



with regularization

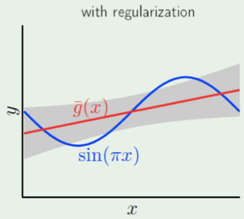
And the winner is ...

without regularization



bias $= \mathbf{0.21}$ var $= \mathbf{1.69}$

with regularization



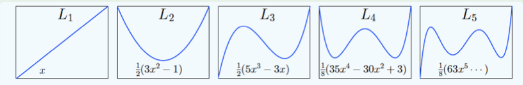
bias $= \mathbf{0.23}$ var $= \mathbf{0.33}$

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

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

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

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

Constraining the weights

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

Softer version: $\sum_{q=0}^{Q} w_q^2 \le C$ "**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 $E_{\text{in}}(\mathbf{w}) = \frac{1}{N} (\mathrm{Z}\mathbf{w} - \mathbf{y})^\intercal (\mathrm{Z}\mathbf{w} - \mathbf{y})$

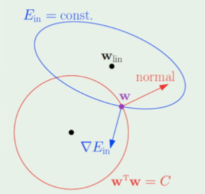
subject to: $\mathbf{w}^\intercal \mathbf{w} \le C$

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

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

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

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



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: $\mathbf{w}^\intercal \mathbf{w} \le C$ $\longleftarrow$ VC formulation

Since some hypothesis are not allowed, we expect the VC dimension to decrease and hence generalization behavior will improve.

The solution

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

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

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

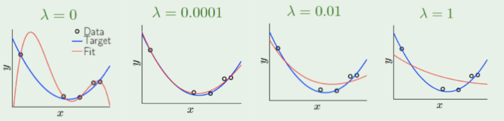
$\boxed{\mathbf{w}_{\text{reg}} = (\mathrm{Z}^\intercal \mathrm{Z} + \lambda \mathrm{I})^{-1} \mathrm{Z}^\intercal \mathbf{y}}$ (with regularization)

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

If λ is large, then we wil have $\frac{1}{\lambda}$ on the right hand side and w will be pıshed towards zero → strong regularization.

The result

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



overfitting $\longrightarrow$ $\longrightarrow$ $\longrightarrow$ $\longrightarrow$ underfitting

Weight 'decay'

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

Gradient descent:

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

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

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

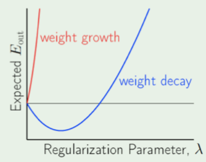
$\gamma_q = 2^{-q} \implies$ high-order fit

Neural networks: different layers get different γ's

Tikhonov regularizer: $\mathbf{w}^{\intercal}\Gamma^{\intercal}\Gamma\mathbf{w}$

Even weight growth!

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



Practical rule:

stochastic noise is 'high-frequency'

deterministic noise is also non-smooth

$\implies$ 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? $\downarrow\downarrow$

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

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

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

The perfect regularizer Ω

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

Guiding principle:

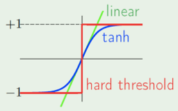
Direction of **smoother** or "simpler"

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

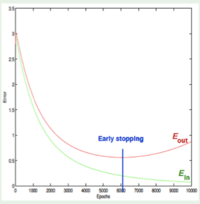
Soft weight elimination:

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

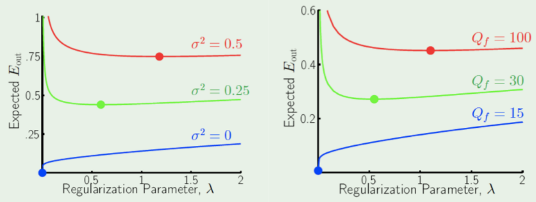
Early stopping as a regularizer

Regularization through the optimizer!

When to stop? **validation**



The optimal λ



Stochastic noise

Deterministic noise