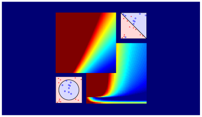
Machine Learning Foundations
(機器學習基石)



Lecture 14: Regularization

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Roadmap

1. When Can Machines Learn?
2. Why Can Machines Learn?
3. How Can Machines Learn?
4. How Can Machines Learn **Better**?

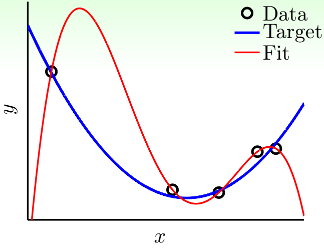
Lecture 13: Hazard of Overfitting

overfitting happens with **excessive power**, **stochastic/deterministic noise**, and **limited data**

Lecture 14: Regularization

- Regularized Hypothesis Set
- Weight Decay Regularization
- Regularization and VC Theory
- General Regularizers

Regularization: The Magic



overfit

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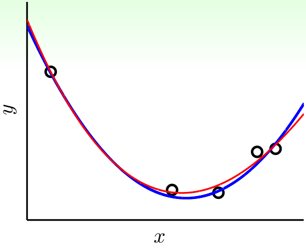
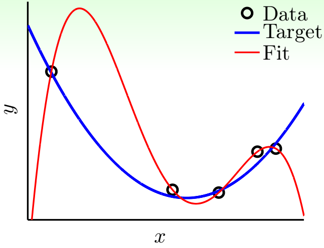


'regularized fit' ⟸ overfit



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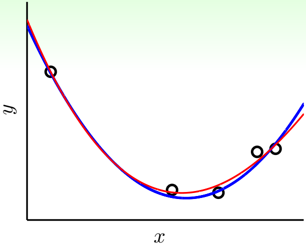

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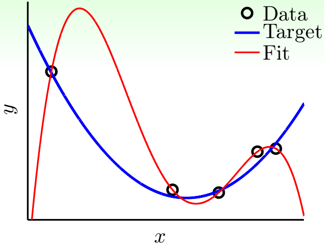
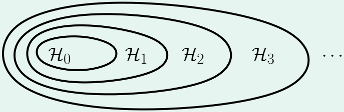


- idea: 'step back' from $\mathcal{H}_{10}$ to $\mathcal{H}_2$



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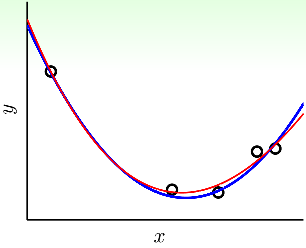

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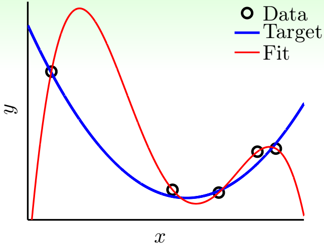

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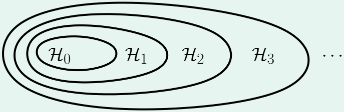

- name history: function approximation for **ill-posed problems**

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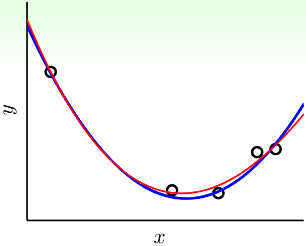

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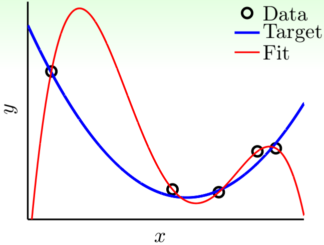

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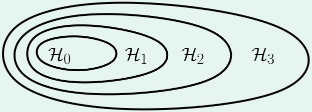
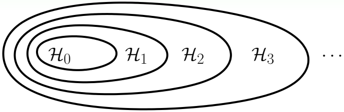


- name history: function approximation for **ill-posed problems**

how to step back?

Stepping Back as Constraint



Q-th order polynomial transform for $x \in \mathbb{R}$:

$$\mathbf{\Phi}_Q(x) = \left(1, x, x^2, \ldots, x^Q\right)$$

+ linear regression, denote $\tilde{\mathbf{w}}$ by $\mathbf{w}$

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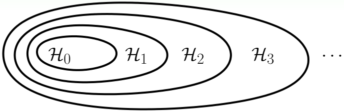

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hypothesis $\mathbf{w}$ in $\mathcal{H}_{10}$: $w_0 + w_1 x + w_2 x^2 + w_3 x^3 + \ldots + w_{10} x^{10}$

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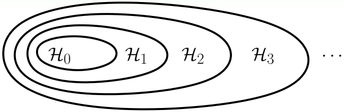

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that is, $\mathcal{H}_2$ = $\mathcal{H}_{10}$ AND 'constraint that $w_3 = w_4 = \ldots = w_{10} = 0$'

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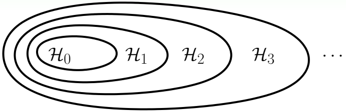

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step back = **constraint**

Regression with Constraint

$$\mathcal{H}_{10} \equiv \left\{ \mathbf{w} \in \mathbb{R}^{10+1} \right\}$$

regression with $\mathcal{H}_{10}$:

$$\min_{\mathbf{w} \in \mathbb{R}^{10+1}} E_{\text{in}}(\mathbf{w})$$

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why don't you just use $\mathbf{w} \in \mathbb{R}^{2+1}$? **:-)**

Regression with Looser Constraint

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- more flexible than $\mathcal{H}_2$: $\mathcal{H}_2 \subset \mathcal{H}_2'$
- less risky than $\mathcal{H}_{10}$: $\mathcal{H}_2' \subset \mathcal{H}_{10}$

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bad news for sparse hypothesis set $\mathcal{H}'_2$:
NP-hard to solve :-(

Regression with Softer Constraint

$$\mathcal{H}_2' \equiv \left\{ \mathbf{w} \in \mathbb{R}^{10+1} \text{ while } \geq 8 \text{ of } w_q = 0 \right\}$$

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$$\mathcal{H}(C) \equiv \left\{ \mathbf{w} \in \mathbb{R}^{10+1} \text{ while } \|\mathbf{w}\|^2 \leq C \right\}$$

regression with $\mathcal{H}(C)$:

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- $\mathcal{H}(C)$: overlaps but not exactly the same as $\mathcal{H}'_2$
- soft and smooth structure over $C \geq 0$:
  $\mathcal{H}(0) \subset \mathcal{H}(1.126) \subset \ldots \subset \mathcal{H}(1126) \subset \ldots \subset \mathcal{H}(\infty) = \mathcal{H}_{10}$

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regularized hypothesis $\mathbf{w}_{\text{REG}}$:
optimal solution from
regularized hypothesis set $\mathcal{H}(C)$

Fun Time

For $Q \geq 1$, which of the following hypothesis (weight vector $\mathbf{w} \in \mathbb{R}^{Q+1}$) is not in the regularized hypothesis set $\mathcal{H}(1)$?

1. $\mathbf{w}^T = [0, 0, \ldots, 0]$
2. $\mathbf{w}^T = [1, 0, \ldots, 0]$
3. $\mathbf{w}^T = [1, 1, \ldots, 1]$
4. $\mathbf{w}^T = \left[\sqrt{\frac{1}{Q+1}}, \sqrt{\frac{1}{Q+1}}, \ldots, \sqrt{\frac{1}{Q+1}}\right]$

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Reference Answer: 3

The squared length of $\mathbf{w}$ in 3 is $Q+1$, which is not ≤ 1.

Matrix Form of Regularized Regression Problem

$$\min_{\mathbf{w} \in \mathbb{R}^{Q+1}} \quad E_{\text{in}}(\mathbf{w}) = \frac{1}{N} \underbrace{\sum_{n=1}^{N} (\mathbf{w}^T \mathbf{z}_n - y_n)^2}$$

$$\text{s.t.} \quad \sum_{q=0}^{Q} w_q^2 \leq C$$

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- $\sum_n \ldots = (\mathrm{Z}\mathbf{w} - \mathbf{y})^T(\mathrm{Z}\mathbf{w} - \mathbf{y})$, **remember? :-)**

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- $\mathbf{w}^T\mathbf{w} \le C$: feasible **w** within a radius-$\sqrt{C}$ hypersphere

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how to solve
constrained optimization problem?

The Lagrange Multiplier

$$\min_{\mathbf{w} \in \mathbb{R}^{Q+1}} \quad E_{\text{in}}(\mathbf{w}) = \frac{1}{N}(\mathrm{Z}\mathbf{w} - \mathbf{y})^T(\mathrm{Z}\mathbf{w} - \mathbf{y}) \text{ s.t. } \mathbf{w}^T\mathbf{w} \leq C$$

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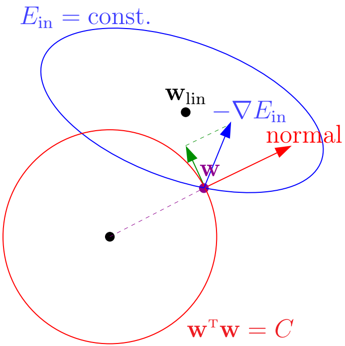

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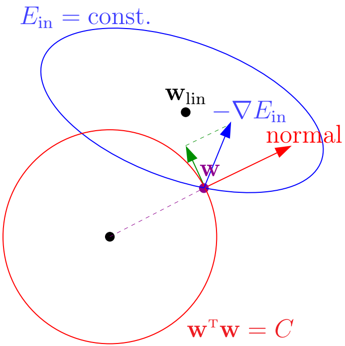

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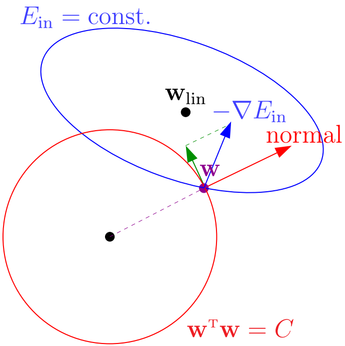

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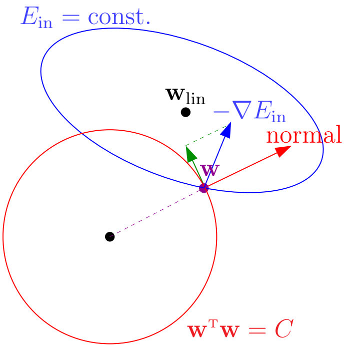
- at optimal solution $\mathbf{w}_{\text{REG}}$, $-\nabla E_{\text{in}}(\mathbf{w}_{\text{REG}}) \propto \boxed{\mathbf{w}_{\text{REG}}}$



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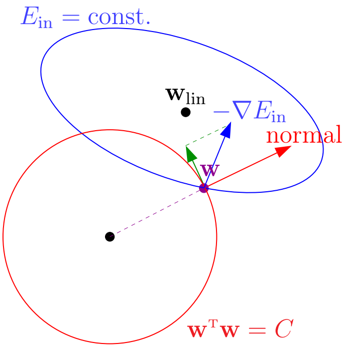

want: find Lagrange multiplier $\lambda > 0$ and $\mathbf{w}_{\text{REG}}$ such that $\nabla E_{\text{in}}(\mathbf{w}_{\text{REG}}) + \frac{2\lambda}{N}\boxed{\mathbf{w}_{\text{REG}}} = \mathbf{0}$

Augmented Error

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

Augmented Error

- if oracle tells you $\lambda > 0$, then

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- optimal solution:

$$\mathbf{w}_{\text{REG}} \leftarrow (Z^T Z + \lambda I)^{-1} Z^T \mathbf{y}$$

—called ridge regression in Statistics

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- regularization with augmented error instead of constrained E_{in}

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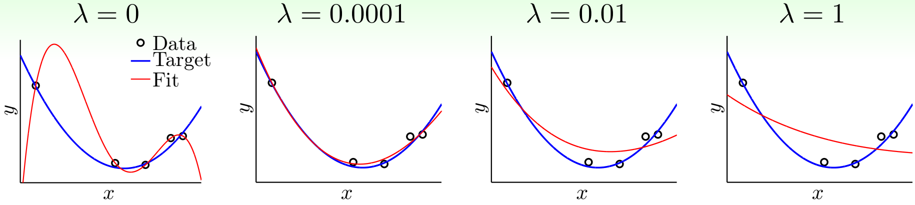
minimizing unconstrained E_{aug} effectively minimizes some C-constrained E_{in}

The Results



overfitting $\Longrightarrow$ $\Longrightarrow$ $\Longrightarrow$ underfitting

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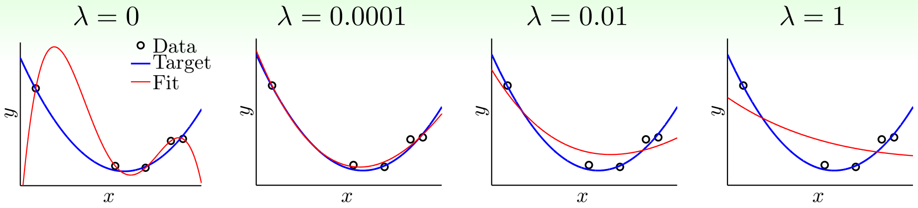

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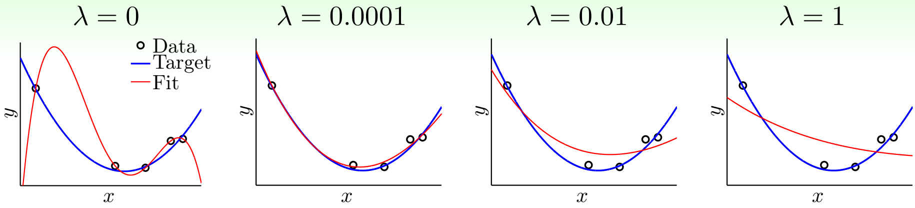

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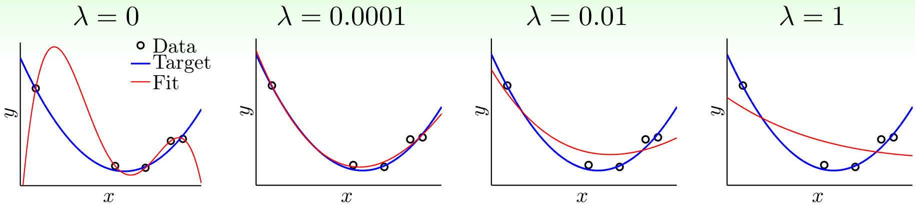

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$\Longleftrightarrow$ prefer shorter $\mathbf{w}$
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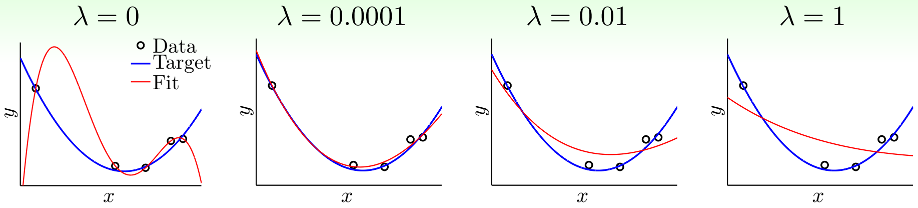

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—go with 'any' transform + linear model

Some Detail: Legendre Polynomials

$$\min_{\mathbf{w}\in\mathbb{R}^{Q+1}} \frac{1}{N}\sum_{n=0}^{N}(\mathbf{w}^T\mathbf{\Phi}(x_n) - y_n)^2 + \frac{\lambda}{N}\sum_{q=0}^{Q} w_q^2$$

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$$\boldsymbol{\Phi}(\mathbf{x}) = (1, x, x^2, \ldots, x^Q)$$

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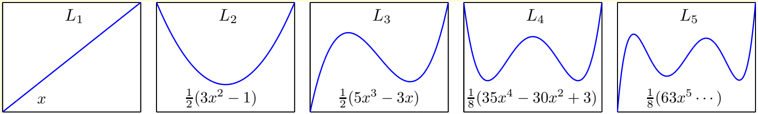
normalized polynomial transform:

$$\left(1, L_1(x), L_2(x), \ldots, L_Q(x)\right)$$

—'orthonormal basis functions' called Legendre polynomials



Fun Time

When would $\mathbf{w}_{\text{REG}}$ equal $\mathbf{w}_{\text{LIN}}$?

1. $\lambda = 0$
2. $C = \infty$
3. $C \geq \|\mathbf{w}_{\text{LIN}}\|^2$
4. all of the above

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Reference Answer: (4)

(1) and (2) shall be easy; (3) means that there are effectively no constraint on **w**, hence the equivalence.

Regularization and VC Theory

Regularization by Constrained-Minimizing E_{in}

$$\min_{\mathbf{w}} E_{\text{in}}(\mathbf{w}) \text{ s.t. } \mathbf{w}^T\mathbf{w} \leq C$$

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minimizing E_{aug}: indirectly getting VC guarantee **without confining to $\mathcal{H}(C)$**

Another View of Augmented Error

Augmented Error

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minimizing E_{aug}:

(heuristically) operating with the better proxy;
(technically) enjoying flexibility of whole $\mathcal{H}$

Effective VC Dimension

$$\min_{\mathbf{w} \in \mathbb{R}^{\tilde{d}+1}} E_{\text{aug}}(\mathbf{w}) = E_{\text{in}}(\mathbf{w}) + \frac{\lambda}{N}\Omega(\mathbf{w})$$

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explanation of regularization:
$d_{\text{VC}}(\mathcal{H})$ large,
while $d_{\text{EFF}}(\mathcal{H}, \mathcal{A})$ small if $\mathcal{A}$ regularized

Fun Time

Consider the weight-decay regularization with regression. When increasing λ in $\mathcal{A}$, what would happen with $d_{\text{EFF}}(\mathcal{H}, \mathcal{A})$?

1. $d_{\text{EFF}} \uparrow$
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4. $d_{\text{EFF}} = 1126$ and does not depend on λ

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Reference Answer: 2

larger λ
$\Longleftrightarrow$ smaller C
$\Longleftrightarrow$ smaller $\mathcal{H}(C)$
$\Longleftrightarrow$ smaller d_{EFF}

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augmented error = error $\widehat{\text{err}}$ + regularizer Ω
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ringing a bell? :-)
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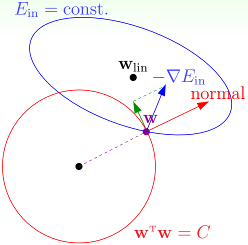
L2 and L1 Regularizer



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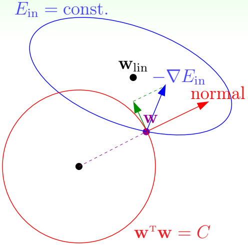

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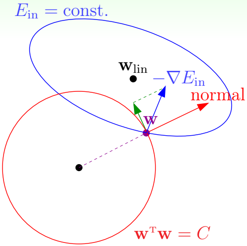

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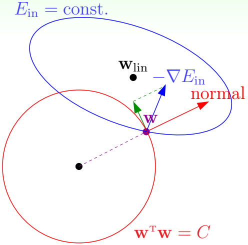

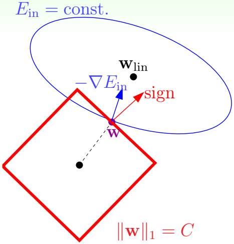

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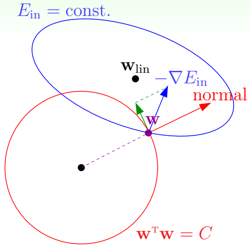

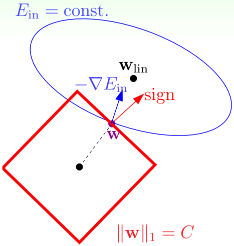

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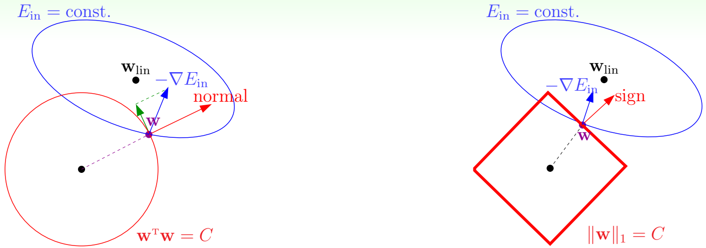

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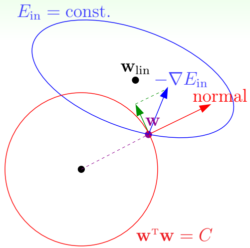

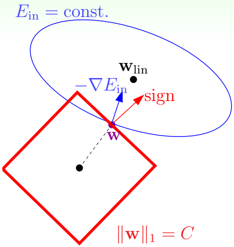

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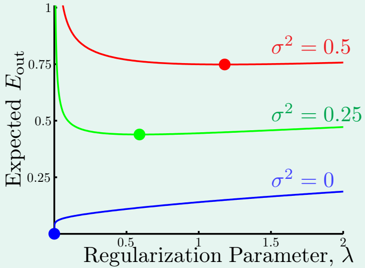
L1 useful if needing **sparse solution**

The Optimal λ

stochastic noise



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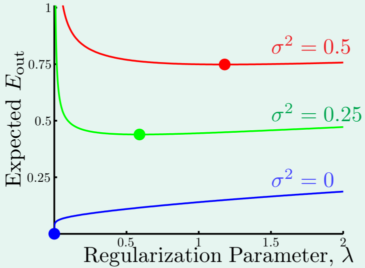

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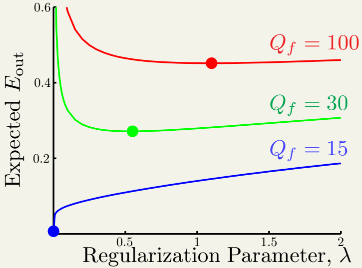

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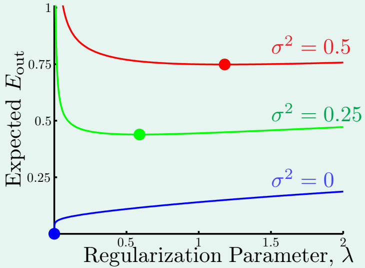

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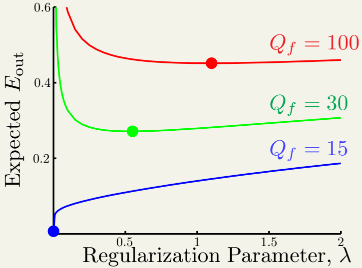

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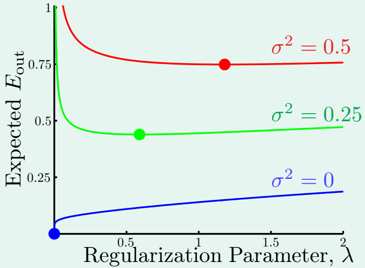

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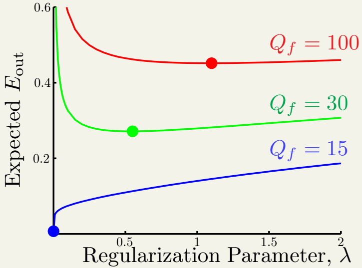

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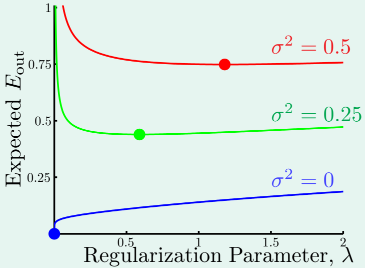

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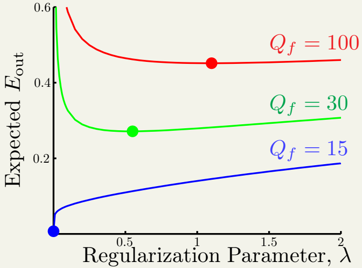

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how to choose?
stay tuned for the next lecture! :-)

Fun Time

Consider using a regularizer $\Omega(\mathbf{w}) = \sum_{q=0}^{Q} 2^q w_q^2$ to work with Legendre polynomial regression. Which kind of hypothesis does the regularizer prefer?

1. symmetric polynomials satisfying $h(x) = h(-x)$
2. low-dimensional polynomials
3. high-dimensional polynomials
4. no specific preference

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Reference Answer: ②

There is a higher 'penalty' for higher-order terms, and hence the regularizer prefers low-dimensional polynomials.

Summary

1. When Can Machines Learn?
2. Why Can Machines Learn?
3. How Can Machines Learn?
4. How Can Machines Learn **Better**?

Lecture 13: Hazard of Overfitting

Lecture 14: Regularization

- Regularized Hypothesis Set
  original $\mathcal{H}$ + constraint
- Weight Decay Regularization
  add $\frac{\lambda}{N}\mathbf{w}^T\mathbf{w}$ in E_{aug}
- Regularization and VC Theory
  regularization decreases d_{EFF}
- General Regularizers
  target-dependent, [plausible], or [friendly]

- **next: choosing from the so-many models/parameters**