COMP5212: Machine Learning

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VC dimension
Definition

- The VC dimension of a hypothesis set $\mathscr{H}$, denoted by $d_{\text{VC}}(\mathscr{H})$, is the largest value of N for which $m_{\mathscr{H}}(N) = 2^N$
  - "The most points $\mathscr{H}$ can shatter"
- $N \leq d_{\text{VC}}(\mathscr{H}) \Rightarrow \mathscr{H}$ can shatter N points
- $k > d_{\text{VC}}(\mathscr{H}) \Rightarrow \mathscr{H}$ cannot be shattered
- The smallest **break point** is 1 above VC-dimension

VC dimension

The growth function

- In terms of a break point k:
  - $m_{\mathscr{H}}(N) \leq \sum_{i=0}^{k-1} \binom{N}{i}$
- In terms of the VC dimension d_{VC}:
  - $m_{\mathscr{H}}(N) \leq \sum_{i=0}^{d_{\text{VC}}} \binom{N}{i}$

VC dimension

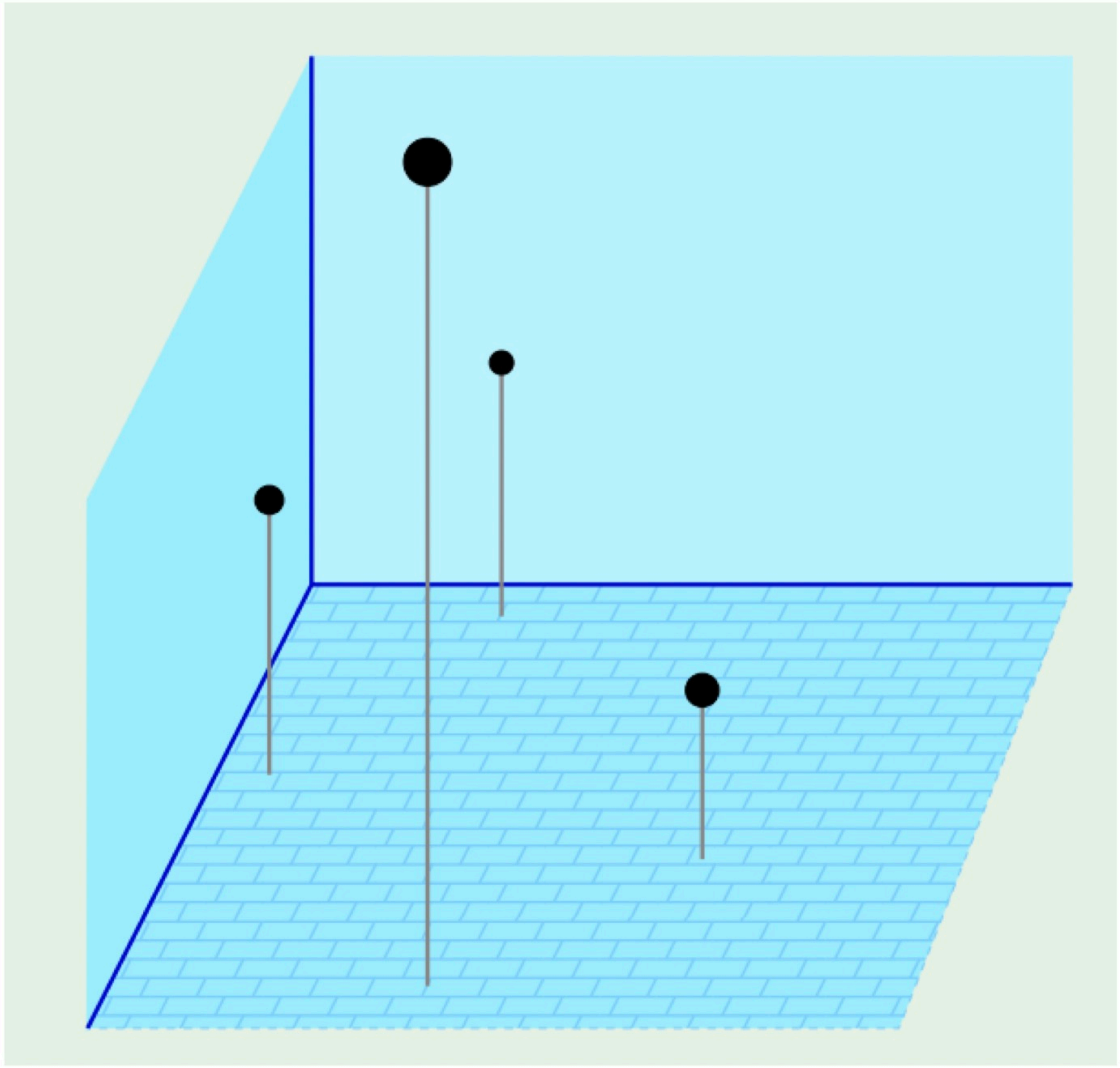
VC dimension of linear classifier

- For $d = 2$, $d_{\text{VC}} = 3$

VC dimension

VC dimension of linear classifier

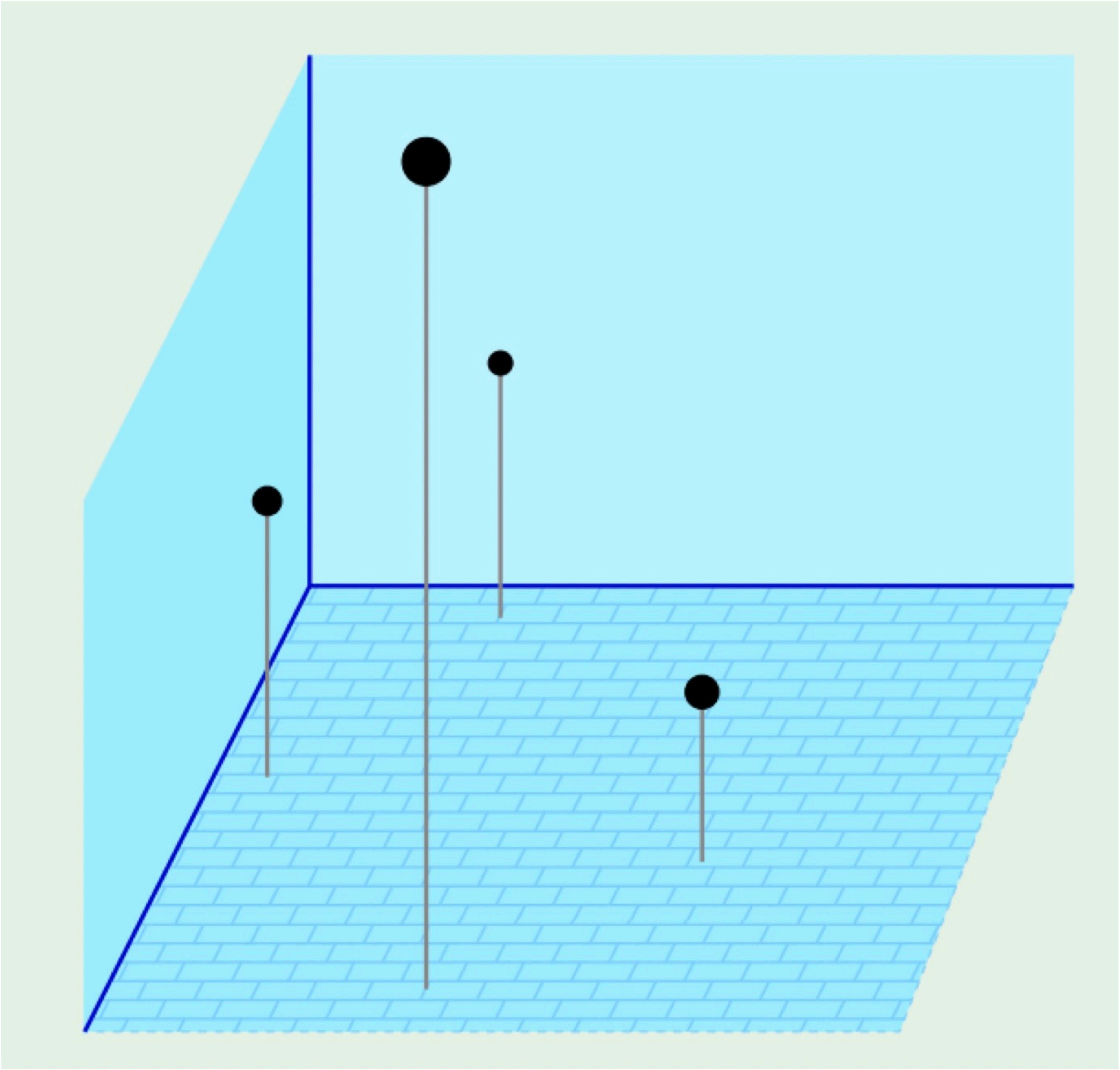
- For $d = 2, d_{\text{VC}} = 3$
- What if $d > 2$?



VC dimension

VC dimension of linear classifier

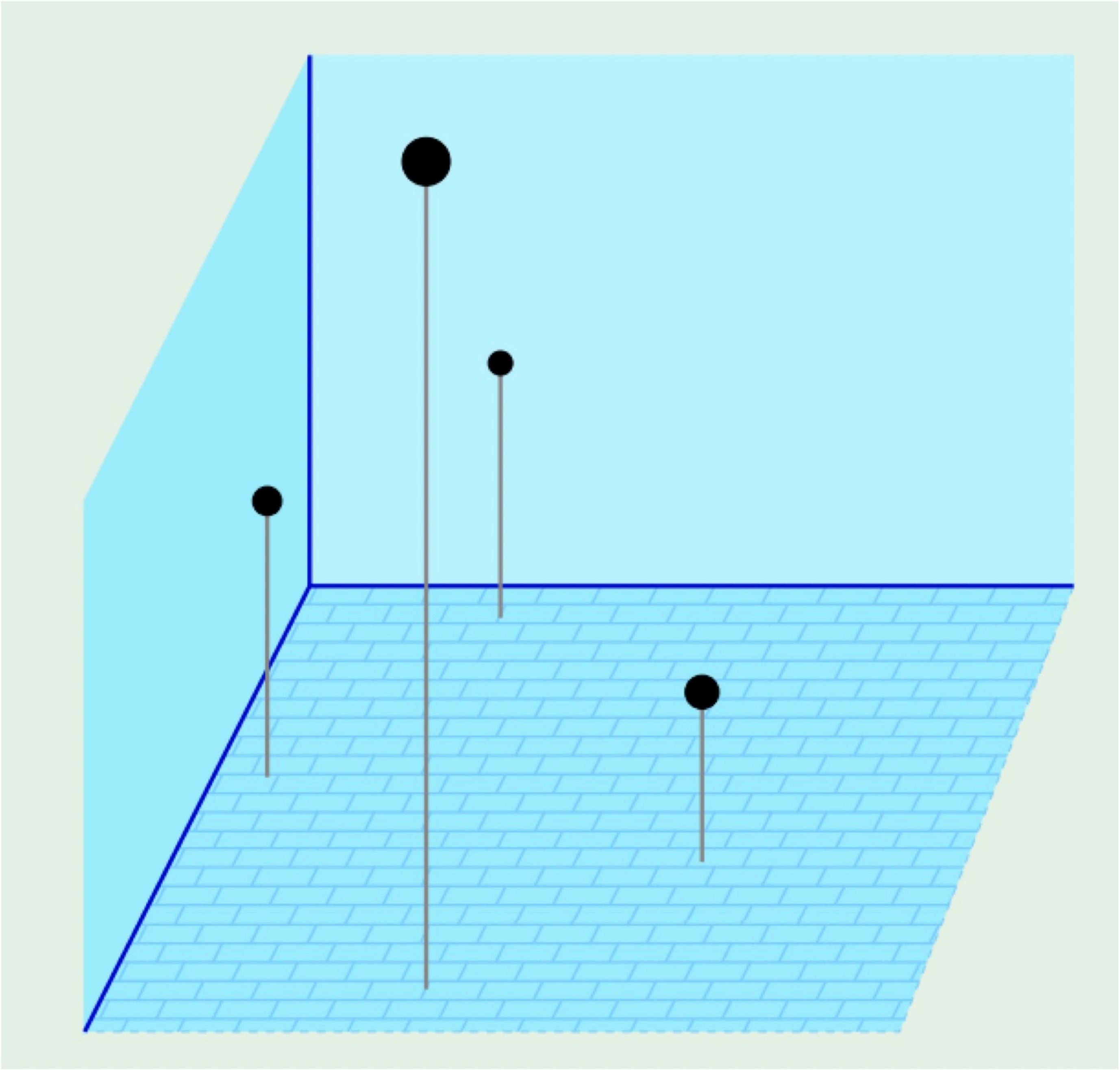
- For $d = 2$, $d_{\text{VC}} = 3$
- What if $d > 2$?
- In general,
  - $d_{\text{VC}} = d + 1$



VC dimension

VC dimension of linear classifier

- For $d = 2$, $d_{\text{VC}} = 3$
- What if $d > 2$?
- In general,
    - $d_{\text{VC}} = d + 1$
- We will prove $d_{\text{VC}} \geq d + 1$ and $d_{\text{VC}} \leq d + 1$



VC dimension

VC dimension of linear classifier

- To prove $d_{\text{VC}} \geq d + 1$

VC dimension

VC dimension of linear classifier

- To prove $d_{\text{VC}} \geq d + 1$
- A set of $N = d + 1$ points in $\mathbb{R}^d$ shattered by the linear hyperplane

$$
\mathrm{X} = \begin{bmatrix} -\ \mathbf{x}_1^\intercal\ - \\ -\ \mathbf{x}_2^\intercal\ - \\ -\ \mathbf{x}_3^\intercal\ - \\ \vdots \\ -\mathbf{x}_{d+1}^\intercal- \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & \ldots & 0 \\ 1 & 1 & 0 & \ldots & 0 \\ 1 & 0 & 1 & & 0 \\ & \vdots & & \ddots & 0 \\ 1 & 0 & \ldots & 0 & 1 \end{bmatrix}
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VC dimension

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- X is invertible!

VC dimension

Can we shatter the dataset?

- For any $y = \begin{bmatrix} y1 \\ y_2 \\ \vdots \\ y_{d+1} \end{bmatrix} = \begin{bmatrix} \pm 1 \\ \pm 1 \\ \vdots \\ \pm 1 \end{bmatrix}$, can be find w satisfying
    - $\text{sign}(Xw) = y$

VC dimension

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VC dimension

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- So, $d_{\text{VC}} \geq d + 1$

VC dimension

VC dimension of linear classifier

- To show $d_{\text{VC}} \leq d + 1$, we need to show
  - We cannot shatter any set of $d + 2$ points

VC dimension

VC dimension of linear classifier

- To show $d_{\text{VC}} \leq d+1$, we need to show
  - We cannot shatter any set of $d+2$ points
- For any $d+2$ points
  - $x_1, x_2, \ldots, x_{d+1}, x_{d+2}$
- More points than dimensions ⇒ linear dependent
  - $x_j = \sum_{i \neq j} a_i x_i$
  - Where not all a_i's are zeros

VC dimension

VC dimension of linear classifier

- $x_j = \sum_{i \neq j} a_i x_i$
- Now we construct a dichotomy that cannot be generated:
  - $y_i = \begin{cases} \text{sign}(a_i) & \text{if } i \neq j \\ -1 & \text{if } i = j \end{cases}$

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  $\text{sign}(a_i) = \text{sign}(w^T x_i) \Rightarrow a_i w^T x_i > 0$

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- Therefore, $y_j = \text{sign}(w^T x_j) = +1$ (cannot be -1)

VC dimension

Putting it together

- We proved for d-dimensional linear hyperplane
  - $d_{\text{VC}} \geq d + 1$ and $d_{\text{VC}} \leq d + 1 \Rightarrow \quad d_{\text{VC}} = d + 1$
- Number of parameters $w_0, \ldots, w_d$
  - $d + 1$ parameters!

VC dimension

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- We proved for d-dimensional linear hyperplane
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- Number of parameters $w_0, \ldots, w_d$
  - $d + 1$ parameters!
- Parameters create degrees of freedom

VC dimension

Number of data points needed

- $$\mathbb{P}[\,|E_{\text{in}}(g) - E_{\text{out}}(g)| > \epsilon] \leq \underbrace{4m_{\mathscr{H}}(2N)e^{-\frac{1}{8}\epsilon^2 N}}_{\delta}$$

- If we want certain ϵ and δ, how does N depend on d_{VC}?

VC dimension

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- Need $N^d e^{-N}$ = small value

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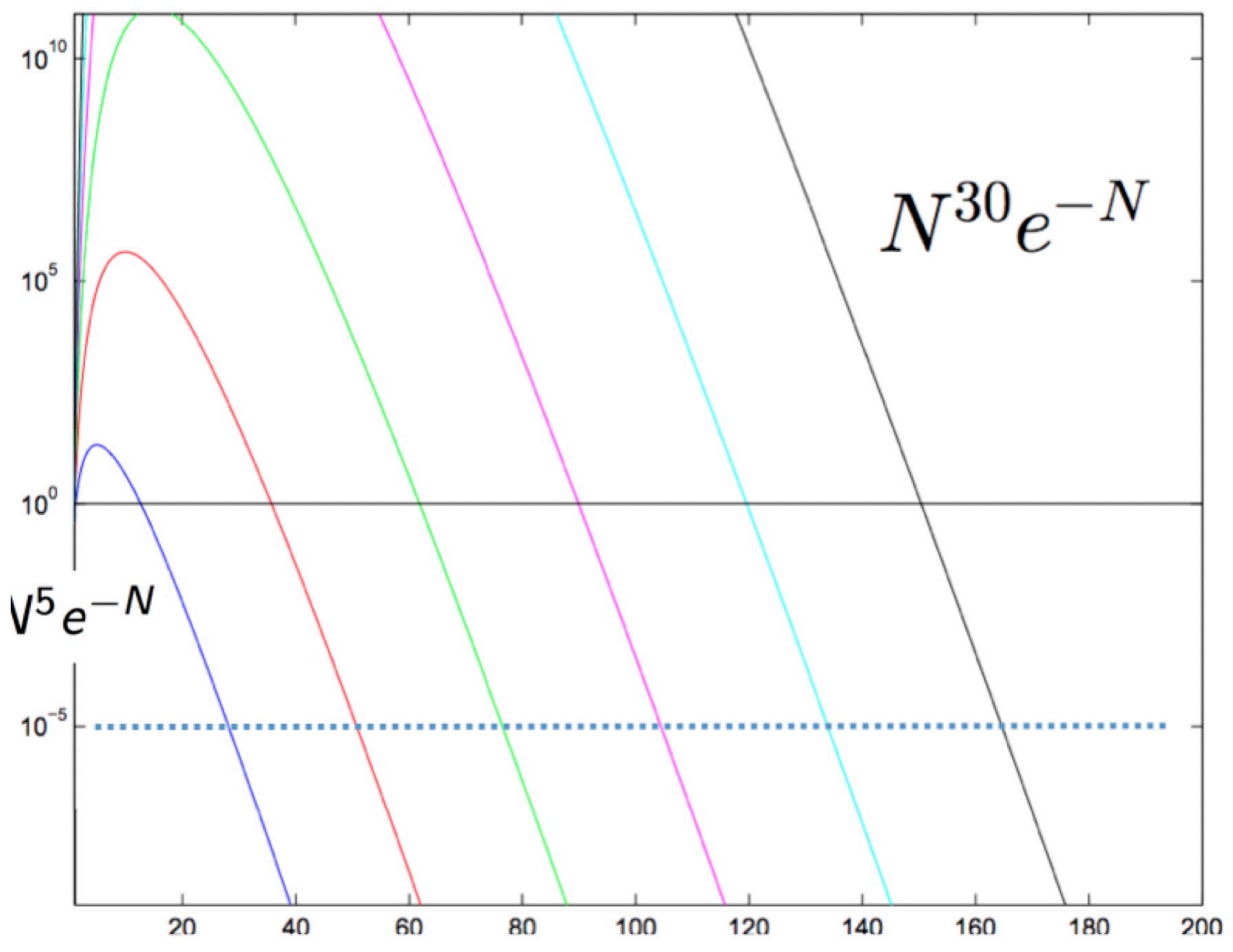


N is almost linear with d_{VC}

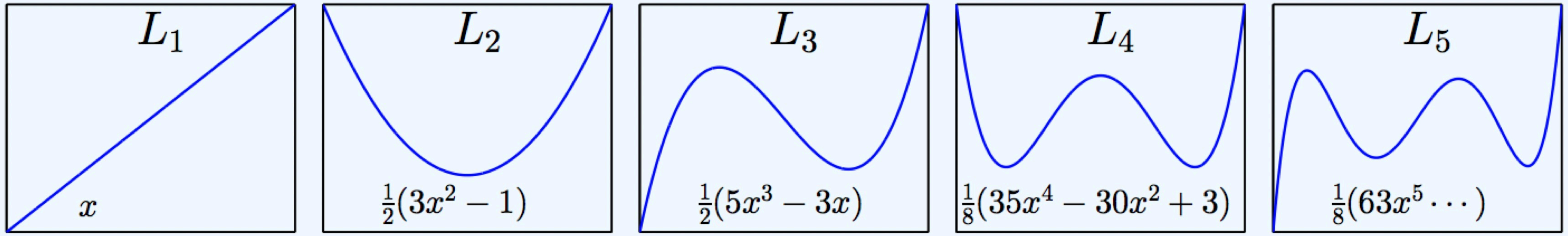
Regularization

Regularization

The polynomial model

- $\mathscr{H}_Q$: polynomials of order Q
    - $\mathscr{H}_Q = \{\sum_{q=0}^{Q} w_q L_q(x)\}$
- Linear regression in the $\mathscr{Z}$ space with
    - $z = [1, L_1(x), \ldots, L_Q(x)]$

Legendre polynomials:



Regularization

Unconstrained solution

- Input $(x_1, y_1), \ldots, (x_N, y_N) \to (z_1, y_1), \ldots, (z_N, y_N)$
- Linear regression:
  - Minimize: $E_{\text{tr}}(w) = \dfrac{1}{N} \displaystyle\sum_{n=1}^{N} (w^T z_n - y_n)^2$
  - Minimize: $\dfrac{1}{N}(Zw - y)^T (Zw - y)$
- Solution $w_{\text{tr}} = (Z^T Z)^{-1} Z^T y$

Regularization

Constraining the weights

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

Regularization

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- Soft-order constraint: $\sum_{q=0}^{Q} w_q^2 \leq C$

Regularization

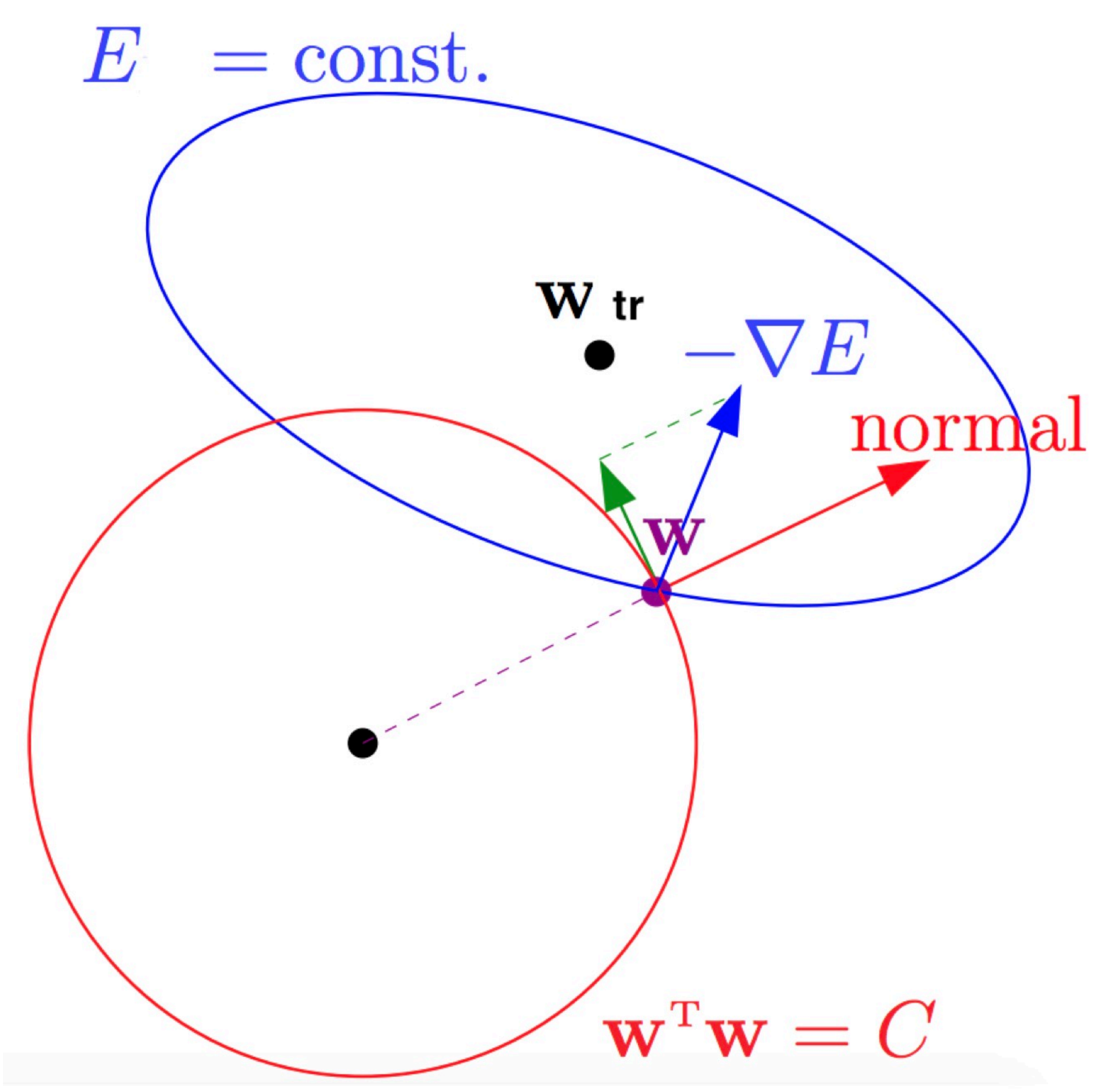
Constraining the weights

- Hard constraint: $\mathscr{H}_2$ is constrained version of $\mathscr{H}_{10}$ (with $w_q = 0$ for $q > 2$)
- Soft-order constraint: $\sum_{q=0}^{Q} w_q^2 \leq C$
- The problem given soft-order constraint:
  - Minimize $\frac{1}{N}(Zw - y)^T(Zw - y)$ s.t. $\underbrace{w^T w \leq C}_{\text{smaller hypothesis space}}$
- Solution w_{reg} instead of w_{tr}

Regularization

Equivalent to the unconstrained version

- Constrained version:
  - $\min_{w} E_{\text{tr}}(w) = \frac{1}{N}(Zw - y)^T(Zw - y)$
    - s.t. $w^T w \leq C$



- Optimal when
  - $\nabla E_{\text{tr}}(w_{\text{reg}}) \propto -w_{\text{reg}}$
  - Why? If $-\nabla E_{\text{tr}}(w_{\text{reg}})$ and w are not parallel, can decrease $E_{\text{tr}}(w)$ without violating the constraint

Regularization

Equivalent to the unconstrained version

- Constrained version:
  - $\min_{w} E_{\text{tr}}(w) = \frac{1}{N}(Zw - y)^T(Zw - y) \quad \text{s.t. } w^T w \leq C$
- Optimal when
  - $\nabla E_{\text{tr}}(w_{\text{reg}}) \propto -w_{\text{reg}}$
- Assume $\nabla E_{\text{tr}}(w_{\text{reg}}) = -2\frac{\lambda}{N}w_{\text{reg}} \Rightarrow \nabla E_{\text{tr}}(w_{\text{reg}}) + 2\frac{\lambda}{N}w_{\text{reg}} = 0$

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- w_{reg} is also the solution of unconstrained problem
  - $\min_{w} E_{\text{tr}}(w) + \frac{\lambda}{N}w^T w$ (Ridge regression!)

Regularization

Equivalent to the unconstrained version

- Constrained version:
  - $\min_{w} E_{\text{tr}}(w) = \frac{1}{N}(Zw - y)^T(Zw - y)$ s.t. $w^T w \leq C$
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- w_{reg} is also the solution of unconstrained problem
  - $\min_{w} E_{\text{tr}}(w) + \frac{\lambda}{N} w^T w$ (Ridge regression!) $C \uparrow$ $\lambda \downarrow$

Regularization

Ridge regression solution

- $\min_w E_{\text{reg}}(w) = \frac{1}{N}\left((Zw - y)^T(Zw - y) + \lambda w^T w\right)$
- $\nabla E_{\text{reg}}(w) = 0 \Rightarrow Z^T Z(w - y) + \lambda w = 0$

Regularization

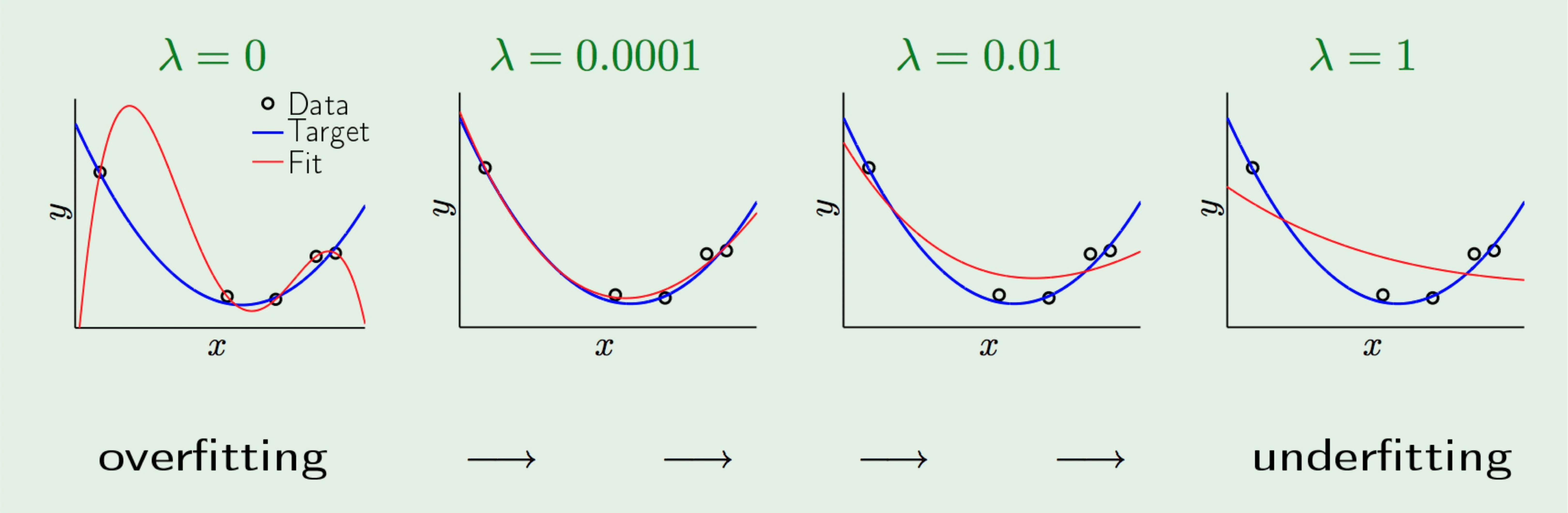
Ridge regression solution

- $\min_{w} E_{\text{reg}}(w) = \dfrac{1}{N}\left((Zw - y)^T(Zw - y) + \lambda w^T w\right)$
- $\nabla E_{\text{reg}}(w) = 0 \Rightarrow Z^T Z(w - y) + \lambda w = 0$
- So, $w_{\text{reg}} = (Z^T Z + \lambda I)^{-1} Z^T y$ (with regularization) as opposed to $w_{\text{tr}} = (Z^T Z)^{-1} Z^T y$ (without regularization)

Regularization

The result

- $\min_{w} E_{\text{tr}}(w) + \frac{\lambda}{N} w^T w$



Regularization

Equivalent to “weight decay”

- Consider the general case
  - $\min_{w} E_{\text{tr}}(w) + \frac{\lambda}{N} w^T w$

Regularization

Equivalent to “weight decay”

- Consider the general case
  - $\min_w E_{\text{tr}}(w) + \frac{\lambda}{N} w^T w$
- Gradient descent:

$$w_{t+1} = w_t - \eta(\nabla E_{\text{tr}}(w_t) + 2\frac{\lambda}{N} w_t)$$

  - $$= w_t \underbrace{(1 - 2\eta\frac{\lambda}{N})}_{\text{weight decay}} - \eta \nabla E_{\text{tr}}(w_t)$$

Regularization

Variations of weight decay

- Emphasis of certain weights:
  - $\sum_{q=0}^{Q} \lambda_q w_q^2$
  - Example 1: $\gamma_q = 2^q \Rightarrow$ low-order fit
  - Example 2: $\gamma_q = 2^{-q} \Rightarrow$ high-order fit

Regularization

Variations of weight decay

- Emphasis of certain weights:
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  - Example 1: $\gamma_q = 2^q \Rightarrow$ low-order fit
  - Example 2: $\gamma_q = 2^{-q} \Rightarrow$ high-order fit
- General Tikhonov regularizer:
  - $w^T H w$ with a positive semi-definite H

Regularization
Variations of weight decay

- Calling the regularizer $\Omega = \Omega(h)$, we minimize
  - $E_{\text{reg}}(h) = E_{\text{tr}}(h) + \frac{\lambda}{N}\Omega(h)$
- In general, $\Omega(h)$ can be any measurement for the "size" of h

Regularization

L2 vs L1 regulariser

- L1-regularizer: $\Omega(w) = \|w\|_1 = \sum_q |w_q|$
- Usually leads to a sparse solution (only few w_q will be nonzero)