Linear classifiers:
Overfitting & regularization

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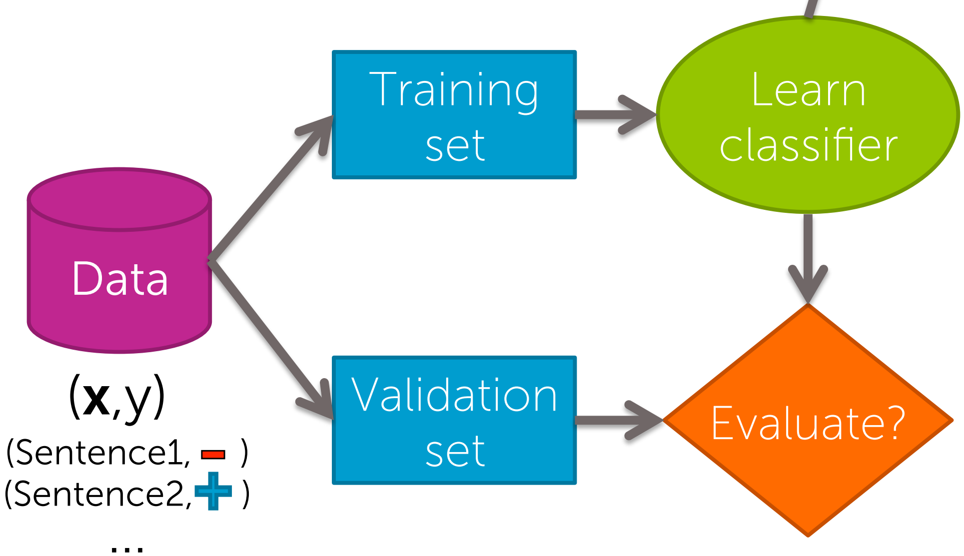
Training and evaluating a classifier

Training a classifier = Learning the coefficients

Word	Coefficient
good	1.0
awesome	1.7
bad	-1.0
awful	-3.3
...	...



Classification error

Learned classifier

$\hat{y} =$ +

Test example

(Sushi was great, +)
(Food was OK, −)

Correct!
Mistake!

Correct	0 / 1
Mistakes	0 / 1

Hide label

Classification error & accuracy

- Error measures fraction of mistakes

$$\text{error} = \frac{\text{\# Mistakes}}{\text{Total number of data points}}$$

  - Best possible value is 0.0

- Often, measure **accuracy**
  - Fraction of correct predictions

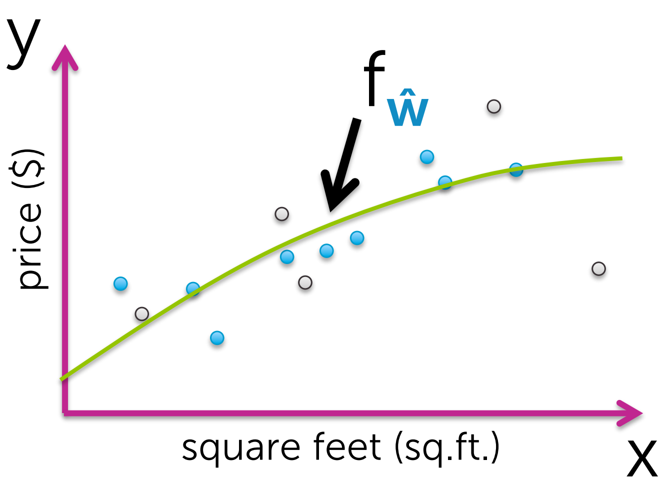
$$\text{accuracy} = \frac{\text{\# Correct}}{\text{Total number of data points}}$$

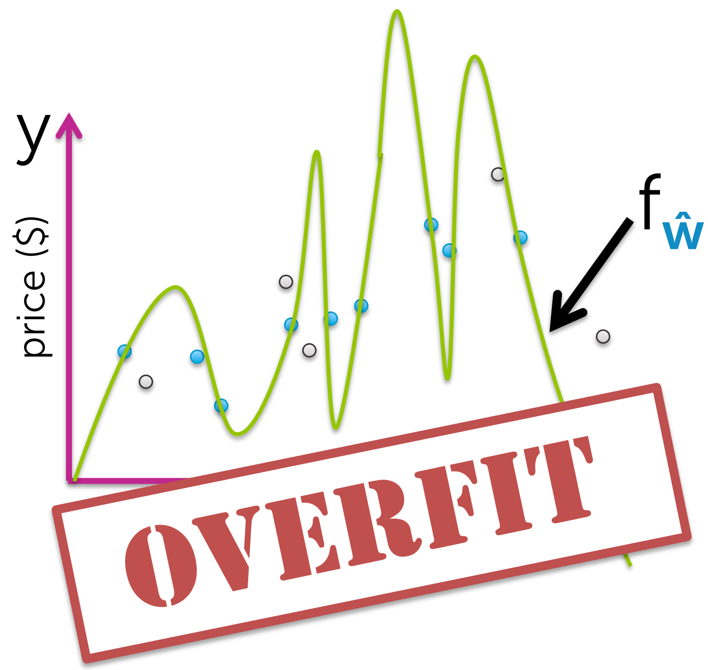
  - Best possible value is 1.0

Overfitting in regression: review

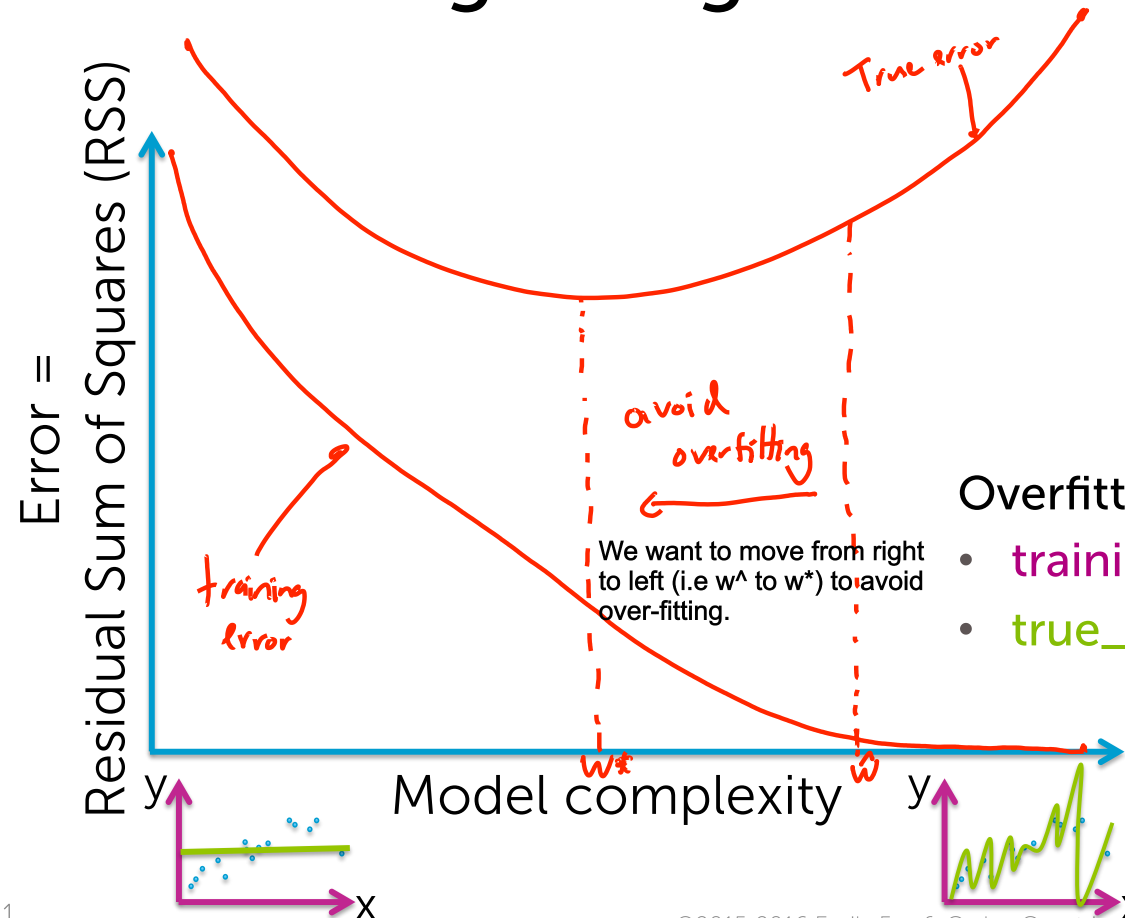
Flexibility of high-order polynomials

$$y_i = w_0 + w_1 x_i + w_2 x_i^2 + \ldots + w_p x_i^p + \varepsilon_i$$





Overfitting in regression



Overfitting if there exists **w***:

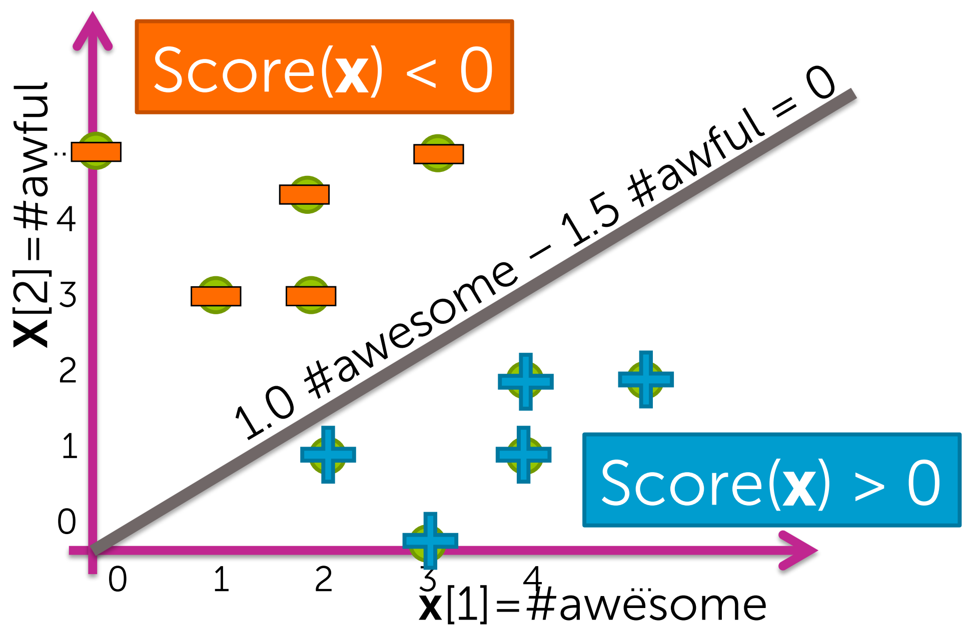
- training_error(**w***) > training_error(**ŵ**)
- true_error(**w***) < true_error(**ŵ**)

Overfitting in classification

Decision boundary example

Word	Coefficient
#awesome	1.0
#awful	-1.5

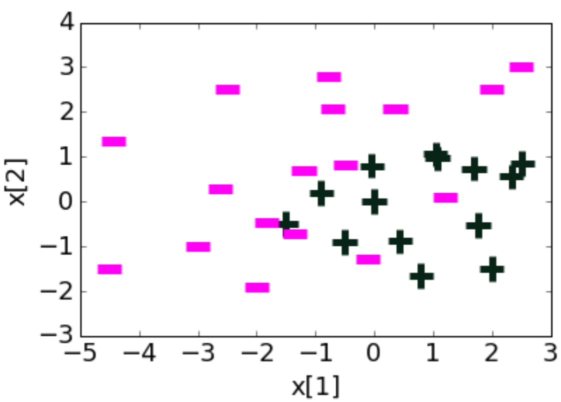
→ Score(x) = 1.0 #awesome – 1.5 #awful

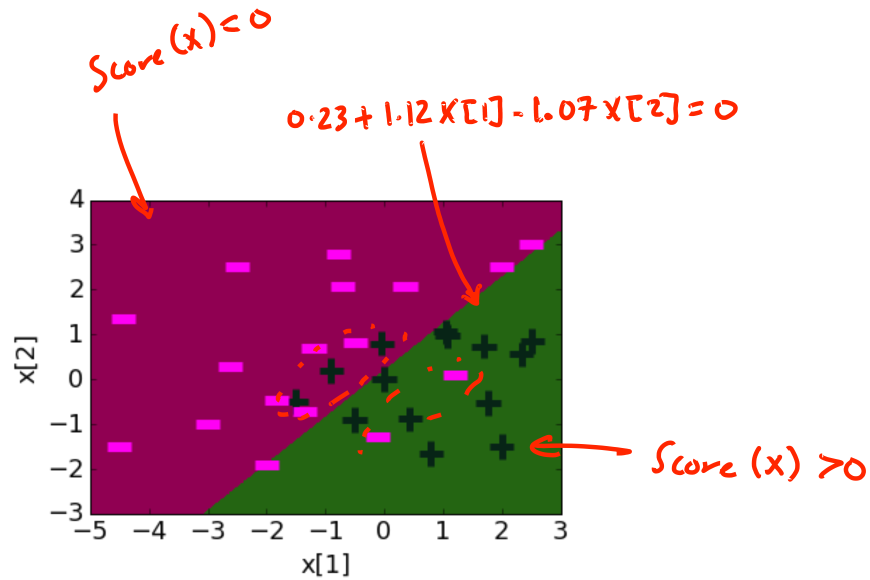


Learned decision boundary

Feature	Value	Coefficient learned
$h_0(\mathbf{x})$	w_0 1	0.23
$h_1(\mathbf{x})$	w_1 $\mathbf{x}[1]$	1.12
$h_2(\mathbf{x})$	w_2 $\mathbf{x}[2]$	−1.07

In this linear classifier some points are misclassified.

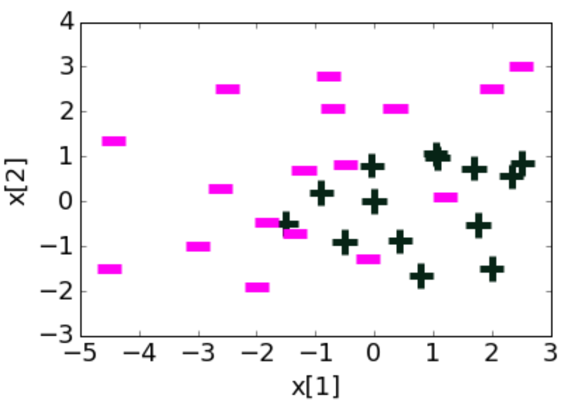




Quadratic features (in 2d)

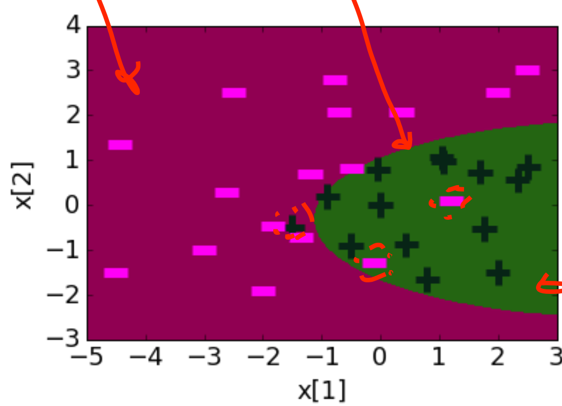
Note: we are not including cross terms for simplicity

Feature	Value	Coefficient learned
$h_0(\mathbf{x})$	1	1.68
$h_1(\mathbf{x})$	$\mathbf{x}[1]$	1.39
$h_2(\mathbf{x})$	$\mathbf{x}[2]$	-0.59
$h_3(\mathbf{x})$	$(\mathbf{x}[1])^2$	-0.17
$h_4(\mathbf{x})$	$(\mathbf{x}[2])^2$	-0.96



Score(x) < 0

$1.68 + 1.39\,x[1] - 0.59\,x[2] - 0.17(x[1])^2 - 0.96(x[2])^2 = 0$



Score(x) > 0

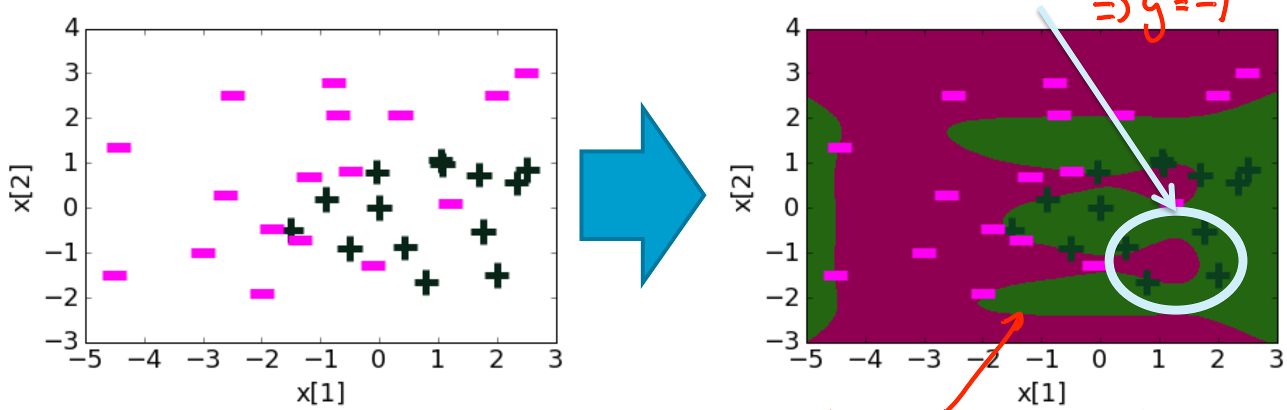
Degree 6 features (in 2d)

Note: we are not including cross terms for simplicity

Feature	Value	Coefficient learned
$h_0(\mathbf{x})$	1	21.6
$h_1(\mathbf{x})$	$\mathbf{x}[1]$	5.3
$h_2(\mathbf{x})$	$\mathbf{x}[2]$	-42.7
$h_3(\mathbf{x})$	$(\mathbf{x}[1])^2$	-15.9
$h_4(\mathbf{x})$	$(\mathbf{x}[2])^2$	-48.6
$h_5(\mathbf{x})$	$(\mathbf{x}[1])^3$	-11.0
$h_6(\mathbf{x})$	$(\mathbf{x}[2])^3$	67.0
$h_7(\mathbf{x})$	$(\mathbf{x}[1])^4$	1.5
$h_8(\mathbf{x})$	$(\mathbf{x}[2])^4$	48.0
$h_9(\mathbf{x})$	$(\mathbf{x}[1])^5$	4.4
$h_{10}(\mathbf{x})$	$(\mathbf{x}[2])^5$	-14.2
$h_{11}(\mathbf{x})$	$(\mathbf{x}[1])^6$	0.8
$h_{12}(\mathbf{x})$	$(\mathbf{x}[2])^6$	-8.6

Coefficient values getting large

Score($\mathbf{x}$) < 0 $\Rightarrow \hat{y} = -1$



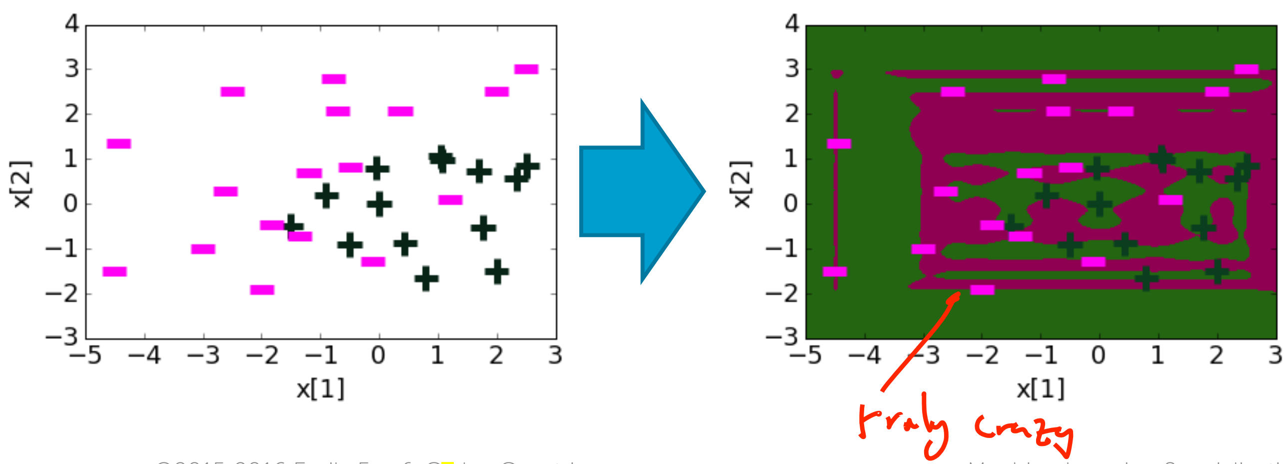
extremely complex (crazy) decision boundary

Degree 20 features (in 2d)

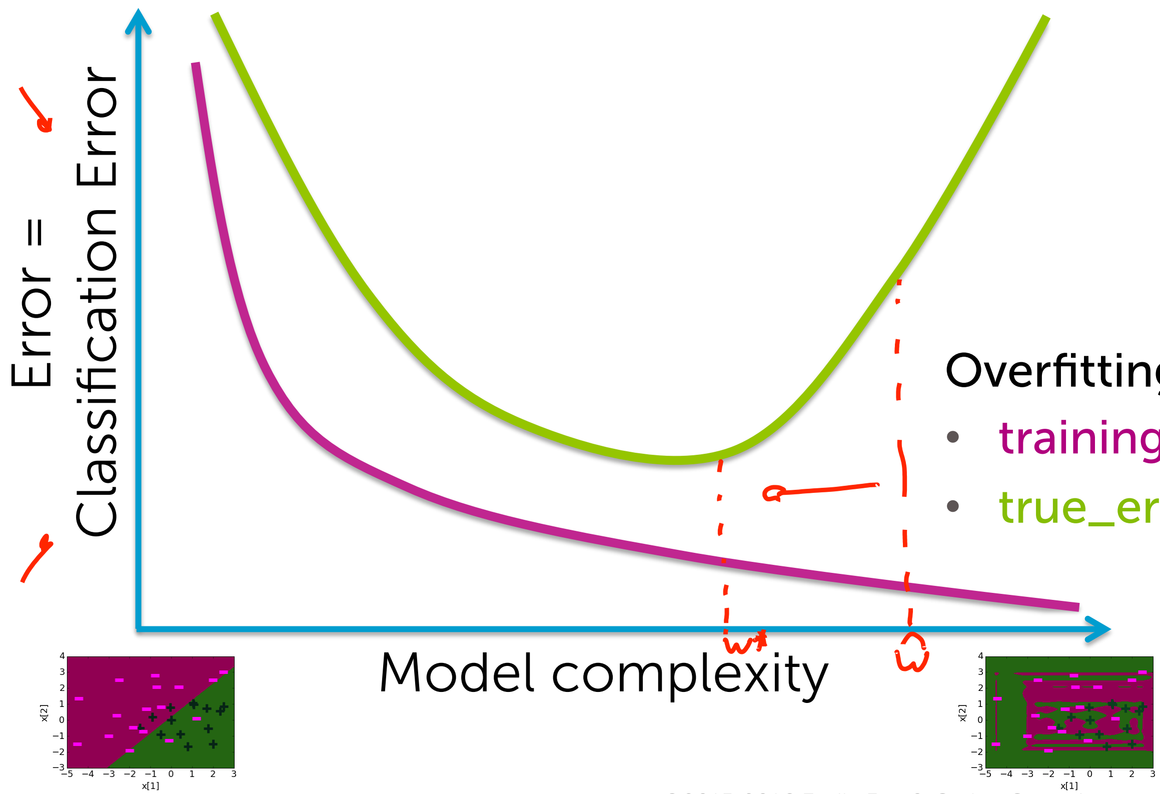
Note: we are not including cross terms for simplicity

Feature	Value	Coefficient learned
$h_0(\mathbf{x})$	1	8.7
$h_1(\mathbf{x})$	$\mathbf{x}[1]$	5.1
$h_2(\mathbf{x})$	$\mathbf{x}[2]$	78.7
…	…	…
$h_{11}(\mathbf{x})$	$(\mathbf{x}[1])^6$	-7.5
$h_{12}(\mathbf{x})$	$(\mathbf{x}[2])^6$	**3803**
$h_{13}(\mathbf{x})$	$(\mathbf{x}[1])^7$	~~21.1~~
$h_{14}(\mathbf{x})$	$(\mathbf{x}[2])^7$	**-2406**
…	…	~~…~~
$h_{37}(\mathbf{x})$	$(\mathbf{x}[1])^{19}$	$-2*10^{-6}$
$h_{38}(\mathbf{x})$	$(\mathbf{x}[2])^{19}$	-0.15
$h_{39}(\mathbf{x})$	$(\mathbf{x}[1])^{20}$	$-2*10^{-8}$
$h_{40}(\mathbf{x})$	$(\mathbf{x}[2])^{20}$	0.03

Often, overfitting associated with very large estimated coefficients $\hat{\mathbf{w}}$



Overfitting in classification

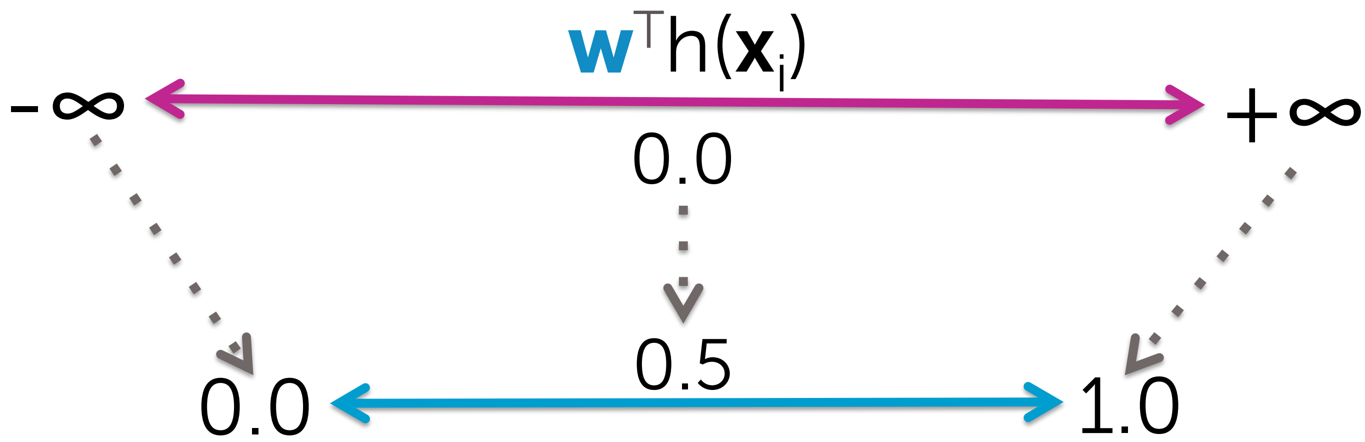


Overfitting if there exists **w***:

- training_error(**w***) > training_error(**ŵ**)
- true_error(**w***) < true_error(**ŵ**)

Overfitting in classifiers → Overconfident predictions

Logistic regression model



$$P(y=+1|\mathbf{x}_i,\mathbf{w}) = \text{sigmoid}(\mathbf{w}^T h(\mathbf{x}_i))$$

The subtle (negative) consequence of overfitting in logistic regression

Overfitting → Large coefficient values

$\hat{\mathbf{w}}^T h(\mathbf{x}_i)$ is very positive (or very negative)
→ **sigmoid**($\hat{\mathbf{w}}^T h(\mathbf{x}_i)$) goes to 1 (or to 0)

Model becomes extremely overconfident of predictions

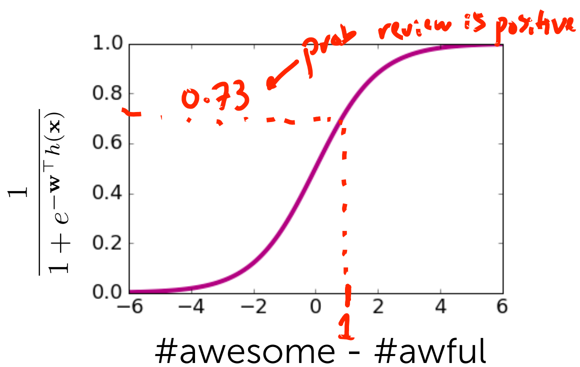
Effect of coefficients on logistic regression model

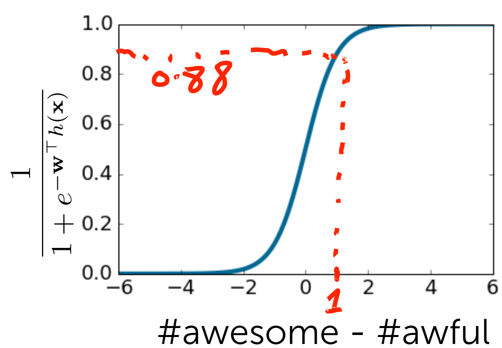
Input x: #awesome=2, #awful=1

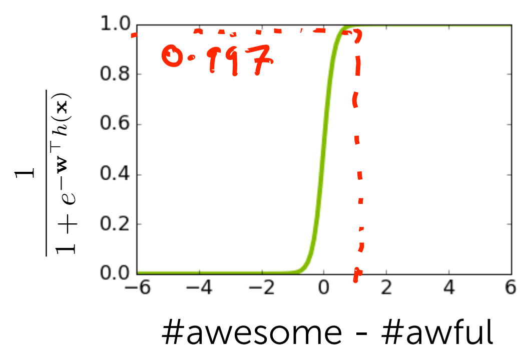
w_0	0
$w_{\#awesome}$	+1
$w_{\#awful}$	-1

w_0	0
$w_{\#awesome}$	+2
$w_{\#awful}$	-2

w_0	0
$w_{\#awesome}$	+6
$w_{\#awful}$	-6







Learned probabilities

Feature	Value	Coefficient learned
$h_0(\mathbf{x})$	1	0.23
$h_1(\mathbf{x})$	$\mathbf{x}[1]$	1.12
$h_2(\mathbf{x})$	$\mathbf{x}[2]$	-1.07

$$P(y=+1 \mid \mathbf{x}, \mathbf{w}) = \frac{1}{1+e^{-\mathbf{w}^\top h(\mathbf{x})}}$$

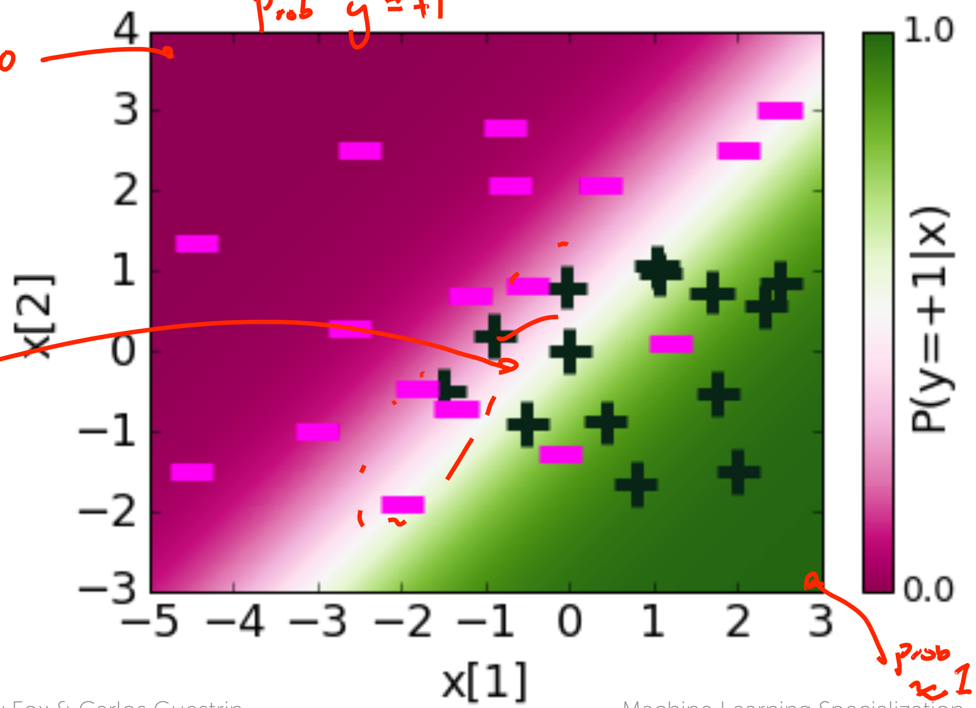
Make sense

wide region of uncertainty

prob ≈ 0.5

prob ≈ 0

Prob $\hat{y}=+1$



prob ≈ 1

Quadratic features: Learned probabilities

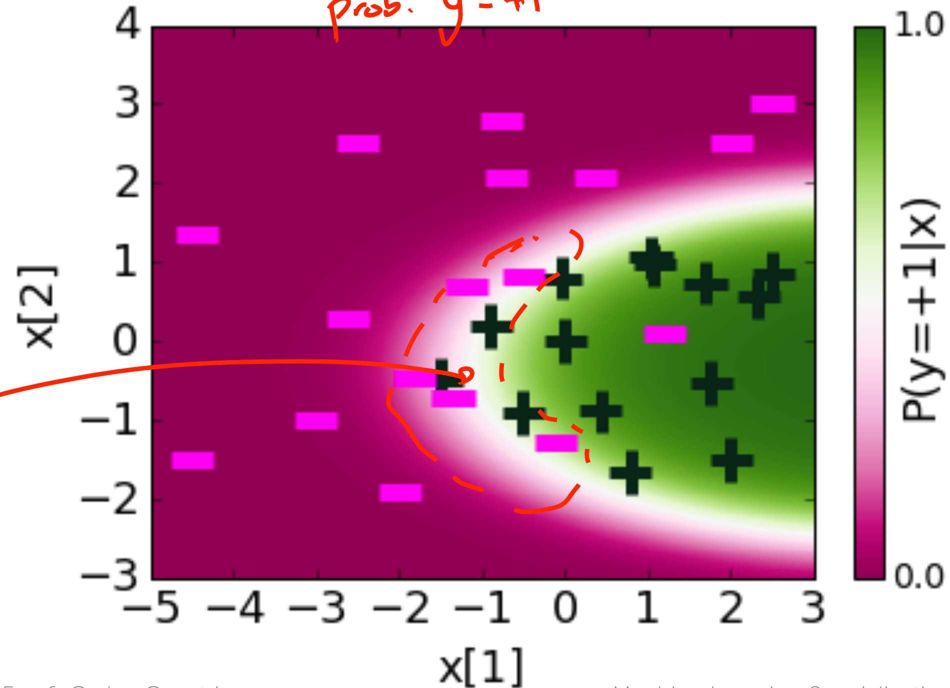
Feature	Value	Coefficient learned
$h_0(\mathbf{x})$	1	1.68
$h_1(\mathbf{x})$	$\mathbf{x}[1]$	1.39
$h_2(\mathbf{x})$	$\mathbf{x}[2]$	-0.58
$h_3(\mathbf{x})$	$(\mathbf{x}[1])^2$	-0.17
$h_4(\mathbf{x})$	$(\mathbf{x}[2])^2$	-0.96

better fit to data

$$P(y=+1 \mid \mathbf{x}, \mathbf{w}) = \frac{1}{1+e^{-\mathbf{w}^\top h(\mathbf{x})}}$$

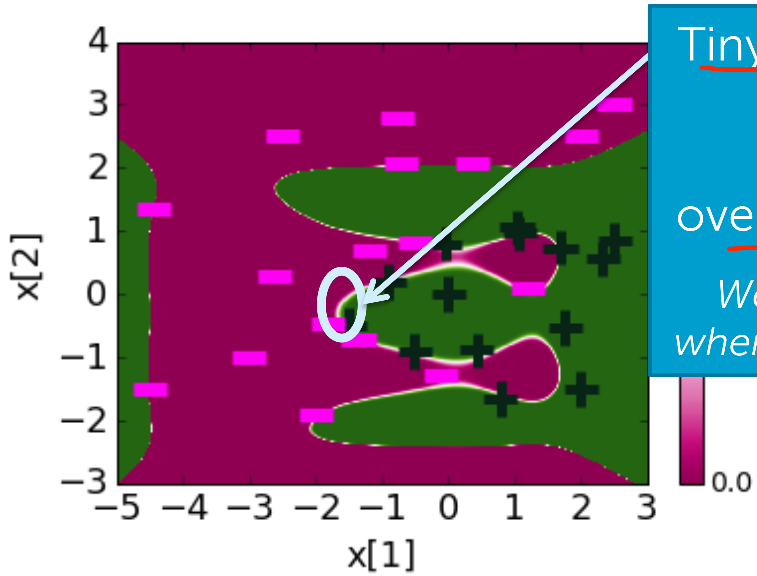
uncertainty region narrower

prob. $\hat{y}=+1$



Overfitting → Overconfident predictions

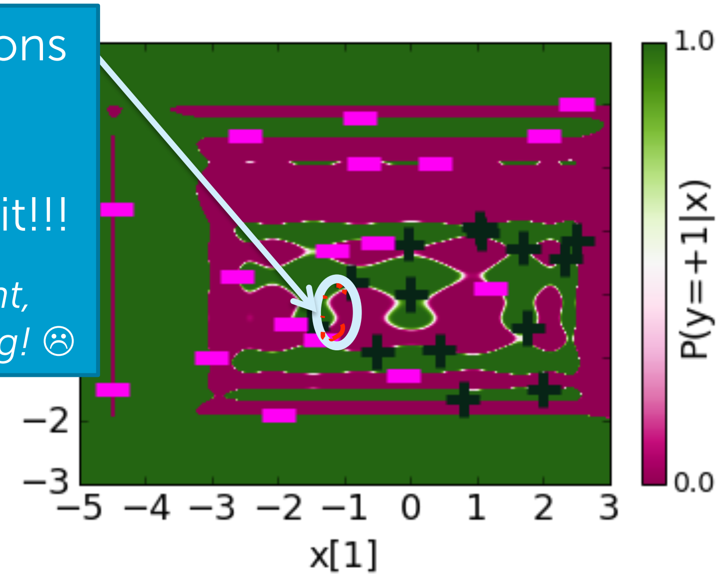
Degree 6: Learned probabilities



Tiny uncertainty regions
→
Overfitting & overconfident about it!!!

We are sure we are right, when we are surely wrong! ☹

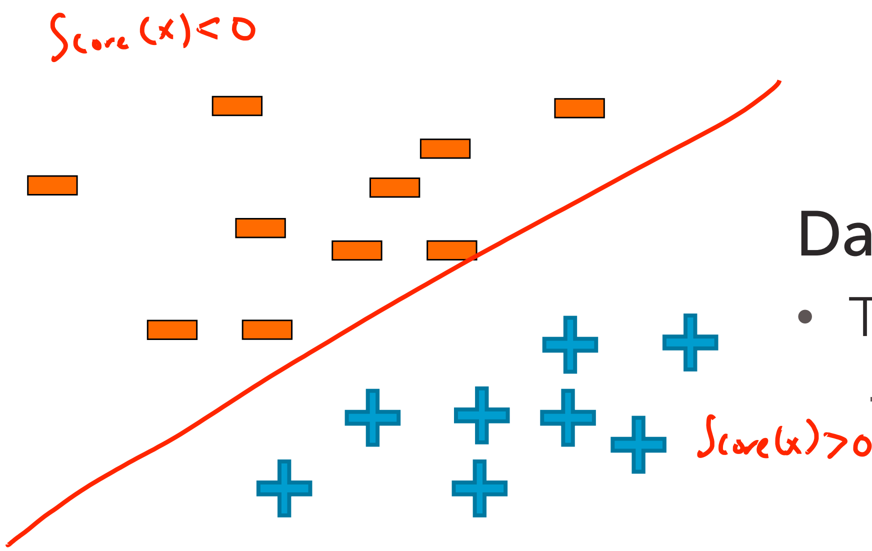
Degree 20: Learned probabilities



Overfitting in logistic regression: Another perspective

OPTIONAL

Linearly-separable data



Data are linearly separable if:

- There exist coefficients $\hat{\mathbf{w}}$ such that:
  - For all positive training data

    $Score(x) = \hat{w}^T h(x) > 0$
  - For all negative training data

    $Score(x) = \hat{w}^T h(x) < 0$

Note 1: If you are using D features, linear separability happens in a D-dimensional space

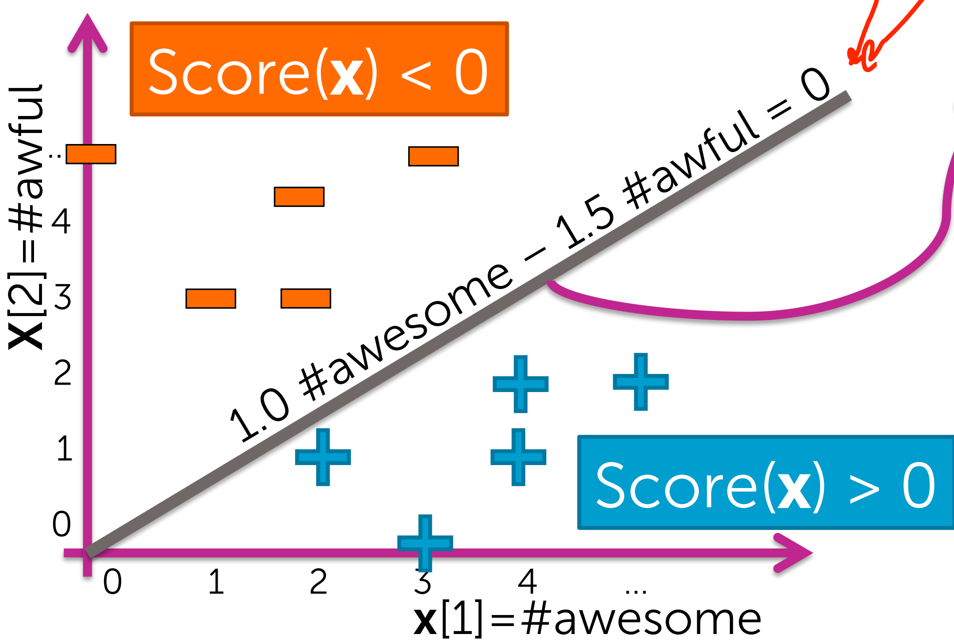
Note 2: If you have enough features, data are (almost) always linearly separable

training_error($\hat{\mathbf{w}}$) = 0

Effect of linear separability on coefficients

1.0 #awesome – 1.5 #awful = 0

10 #awesome – 15 #awful = 0

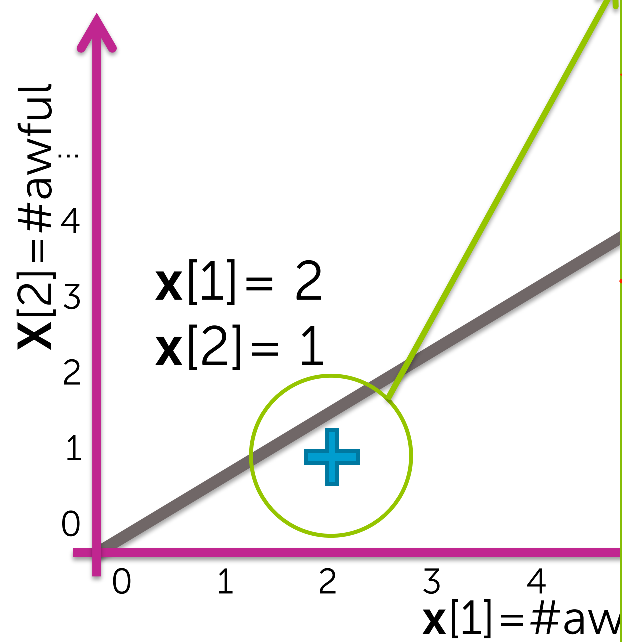


Data are linearly separable with $\hat{w}_1$=1.0 and $\hat{w}_2$=-1.5

Data also linearly separable with $\hat{w}_1$=10 and $\hat{w}_2$=-15

Data also linearly separable with $\hat{w}_1$=10^9 and $\hat{w}_2$=-1.5×10^9

Maximum likelihood estimation (MLE) prefers most certain model → Coefficients go to infinity for linearly-separable data!!!



$P(y=+1 \mid \mathbf{x}_i, \hat{w})$
$\frac{1}{1+e^{-(2-1.5)}} = \frac{1}{1+e^{-0.5}} = 0.62$
$\frac{1}{1+e^{-5}} = 0.99$
$\frac{1}{1+e^{-0.5 \cdot 10^9}} \approx 1$

Data is linearly separable with $\hat{w}_1$=1.0 and $\hat{w}_2$=-1.5

Data also linearly separable with $\hat{w}_1$=10 and $\hat{w}_2$=-15

Data also linearly separable with $\hat{w}_1$=10^9 and $\hat{w}_2$=-1.5x10^9

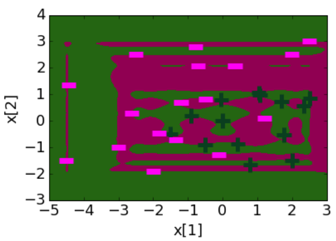
Overfitting in logistic regression is "twice as bad"

Learning tries to find decision boundary that separates data

If data are linearly separable

Overly complex boundary

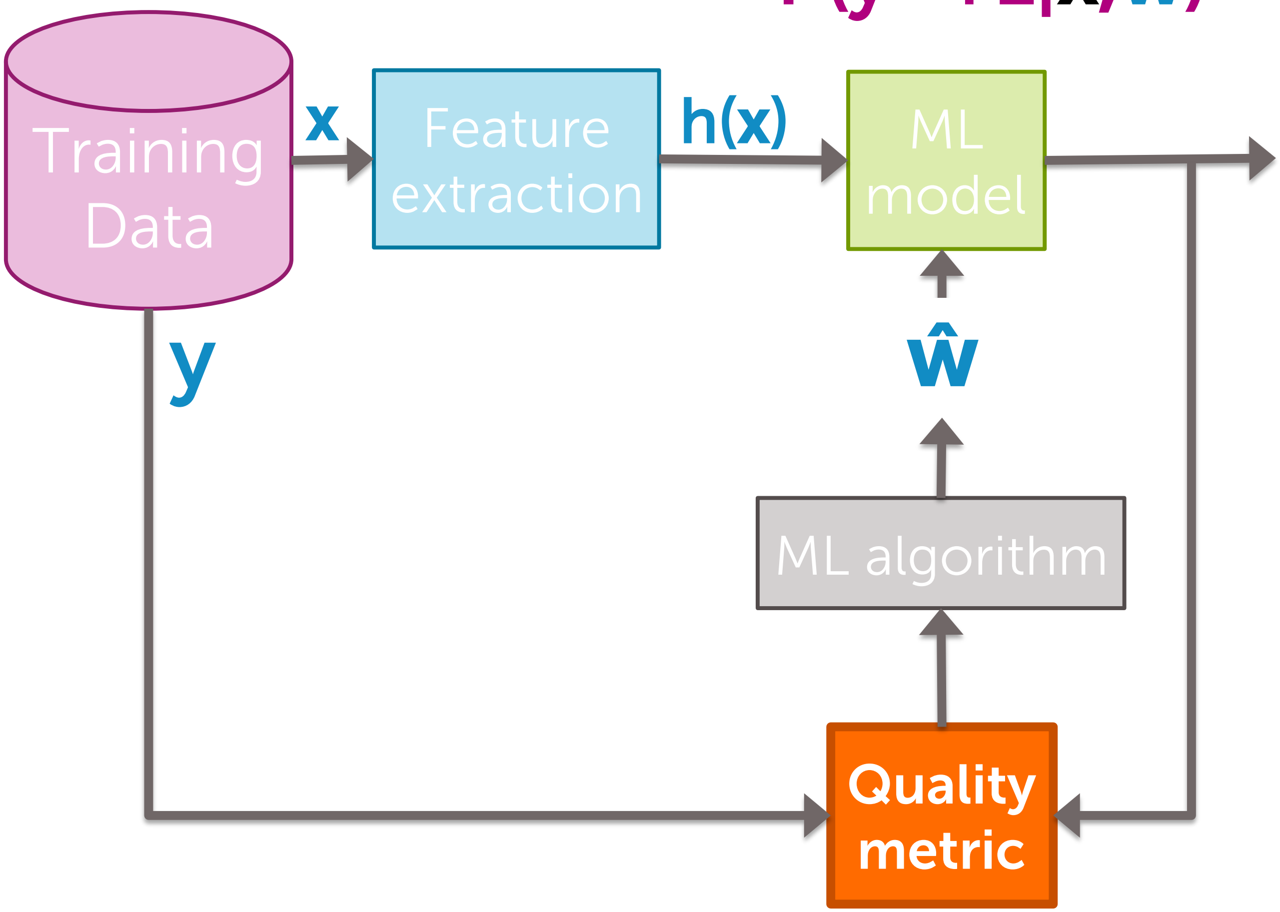
Coefficients go to infinity!



$\hat{w}_1 = 10^9$
$\hat{w}_2 = -1.5\text{x}10^9$

Penalizing large coefficients to mitigate overfitting

$$\hat{P}(y=+1|\mathbf{x},\hat{\mathbf{w}}) = \frac{1}{1+e^{-\hat{\mathbf{w}}^{\top}h(\mathbf{x})}}$$



Desired total cost format

Want to balance:

i. How well function fits data

ii. Magnitude of coefficients

want to balance

Total quality =

measure of fit - measure of magnitude of coefficients

(data likelihood)
large # = good fit to training data

large # = overfit

Maximum likelihood estimation (MLE): Measure of fit = Data likelihood

- Choose coefficients **w** that maximize likelihood:

$$\prod_{i=1}^{N} P(y_i \mid \mathbf{x}_i, \mathbf{w})$$

- Typically, we use the log of likelihood function
(simplifies math and has better convergence properties)

$$\ell(\mathbf{w}) = \ln \prod_{i=1}^{N} P(y_i \mid \mathbf{x}_i, \mathbf{w})$$

Measure of magnitude of logistic regression coefficients

What summary # is indicative of size of logistic regression coefficients?

- Sum of squares (L_2 norm)

$\|w\|_2^2 = w_0^2 + w_1^2 + w_2^2 + \dots + w_D^2$

Penalize large Coefficients

- Sum of absolute value (L_1 norm)

$\|w\|_1 = |w_0| + |w_1| + |w_2| + \dots + |w_D|$

Sparse solution

Consider specific total cost

$$\max_{\mathbf{w}} \text{ Total quality} = \underbrace{\text{measure of fit}}_{\ell(\mathbf{w})} - \underbrace{\text{measure of magnitude of coefficients}}_{||\mathbf{w}||_2^2}$$

log data likelihood

L_2 penalty

Consider resulting objective

What if $\hat{\mathbf{w}}$ selected to minimize

$$\ell(\mathbf{w}) - \lambda||\mathbf{w}||_2^2$$

tuning parameter = balance of fit and magnitude

If λ=0:

Reduces $\max_{w} \ell(w) \rightarrow$ standard (unpenalized) MLE solution

If λ=∞:

$\max_{w} \ell(w) - \infty ||w||_2^2 \rightarrow$ only care about penalizing w, large coefficients $\rightarrow$ $w=0$

If λ in between:

Balance data fit against the magnitude of the coefficients

Consider resulting objective

What if $\hat{\mathbf{w}}$ selected to minimize

$$\ell(\mathbf{w}) - \lambda||\mathbf{w}||_2^2$$

tuning parameter = balance of fit and magnitude

L_2 regularized logistic regression

Pick λ using:
- Validation set (for large datasets)
- Cross-validation (for smaller datasets)

(see regression course)

Bias-variance tradeoff

Large λ:

high bias, low variance

(e.g., $\hat{\mathbf{w}} = 0$ for $\lambda = \infty$)

In essence, λ controls model complexity

Small λ:

low bias, high variance

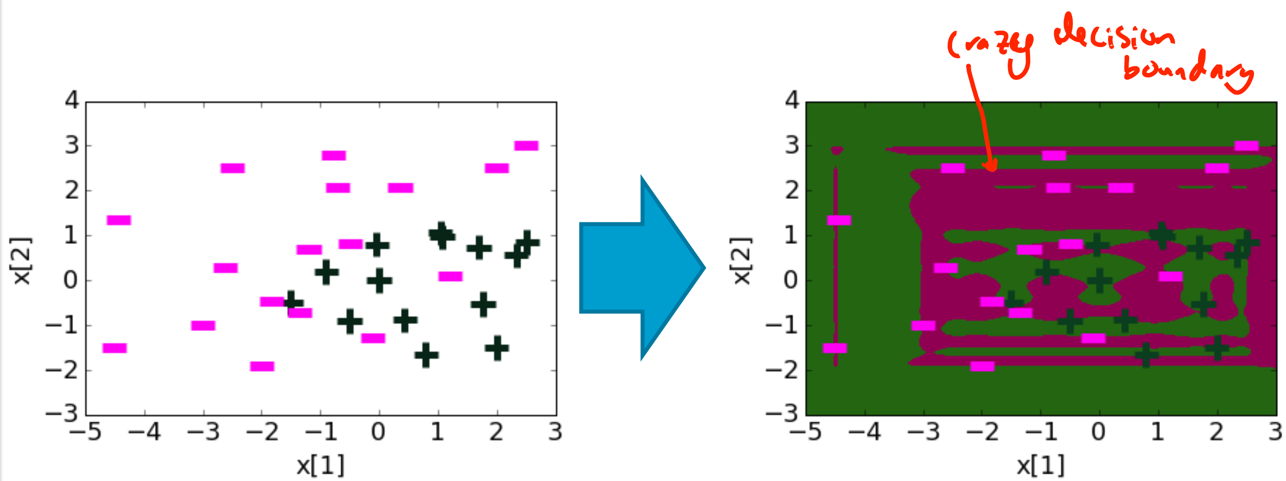
(e.g., maximum likelihood (MLE) fit of high-order polynomial for $\lambda = 0$)

Visualizing effect of regularization on logistic regression

Degree 20 features, $\lambda=0$

Feature	Value	Coefficient learned
$h_0(\mathbf{x})$	1	8.7
$h_1(\mathbf{x})$	$\mathbf{x}[1]$	5.1
$h_2(\mathbf{x})$	$\mathbf{x}[2]$	78.7
…	…	…
$h_{11}(\mathbf{x})$	$(\mathbf{x}[1])^6$	-7.5
$h_{12}(\mathbf{x})$	$(\mathbf{x}[2])^6$	3803
$h_{13}(\mathbf{x})$	$(\mathbf{x}[1])^7$	21.1
$h_{14}(\mathbf{x})$	$(\mathbf{x}[2])^7$	-2406
…	…	…
$h_{37}(\mathbf{x})$	$(\mathbf{x}[1])^{19}$	$-2*10^{-6}$
$h_{38}(\mathbf{x})$	$(\mathbf{x}[2])^{19}$	-0.15
$h_{39}(\mathbf{x})$	$(\mathbf{x}[1])^{20}$	$-2*10^{-8}$
$h_{40}(\mathbf{x})$	$(\mathbf{x}[2])^{20}$	0.03

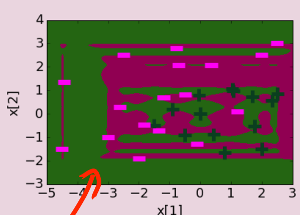
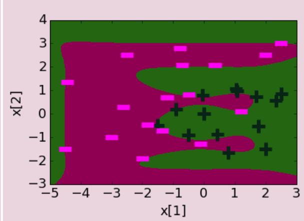
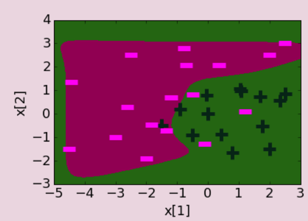
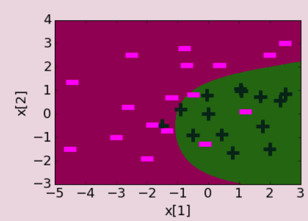
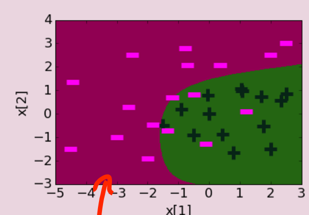
Coefficients range from -3170 to 3803



Degree 20 features, effect of regularization penalty λ

very large

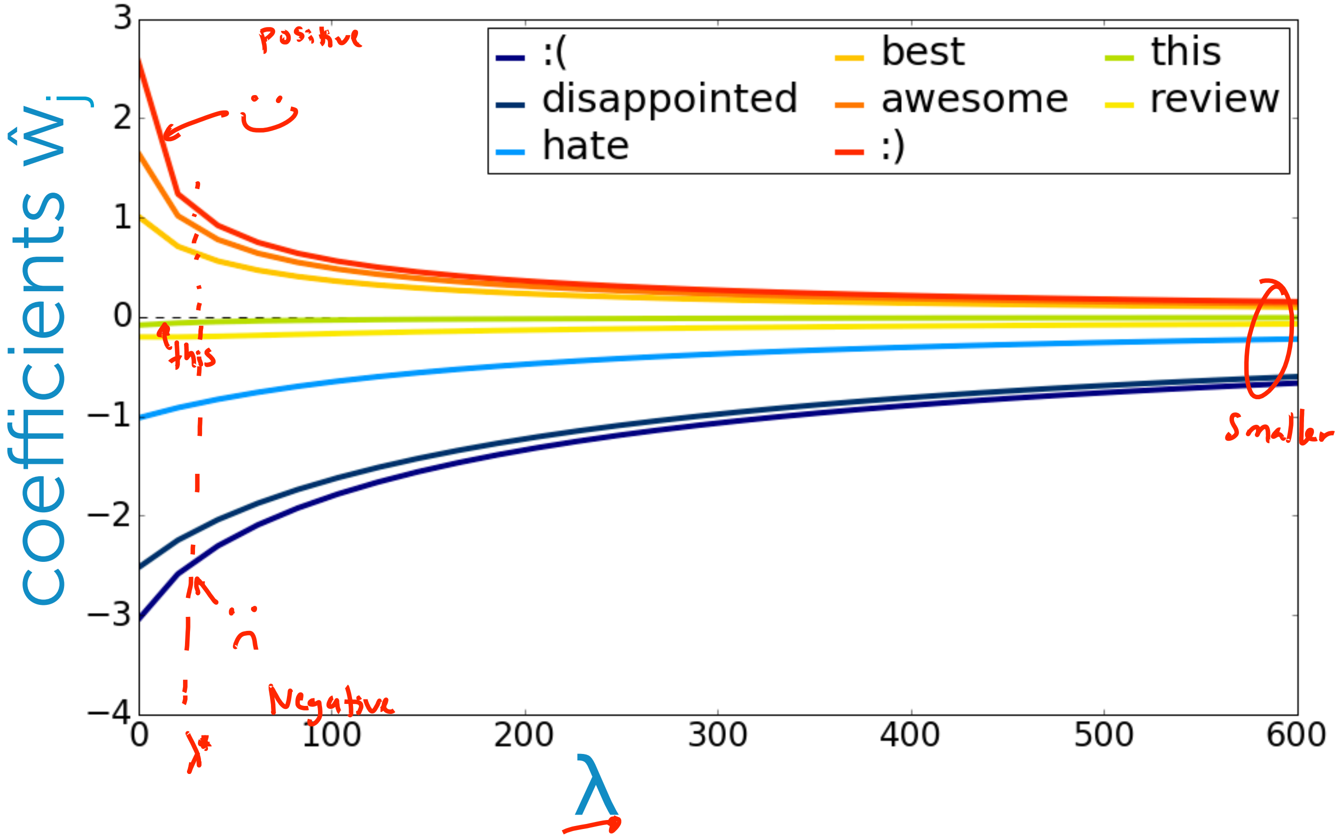
smaller coefficients

Regularization	$\lambda = 0$	$\lambda = 0.00001$	$\lambda = 0.001$	$\lambda = 1$	$\lambda = 10$
Range of coefficients	-3170 to 3803	-8.04 to 12.14	-0.70 to 1.25	-0.13 to 0.57	-0.05 to 0.22
Decision boundary					

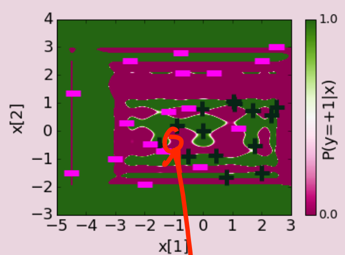
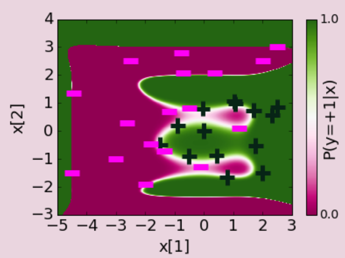
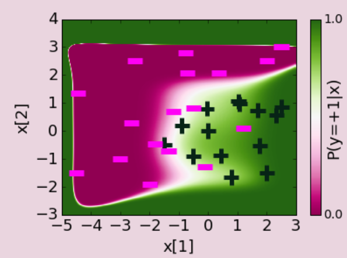
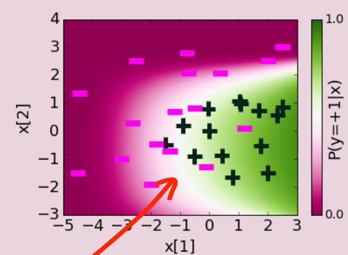
crazy decision boundary

nicer smoother

Coefficient path



Degree 20 features: regularization reduces "overconfidence"

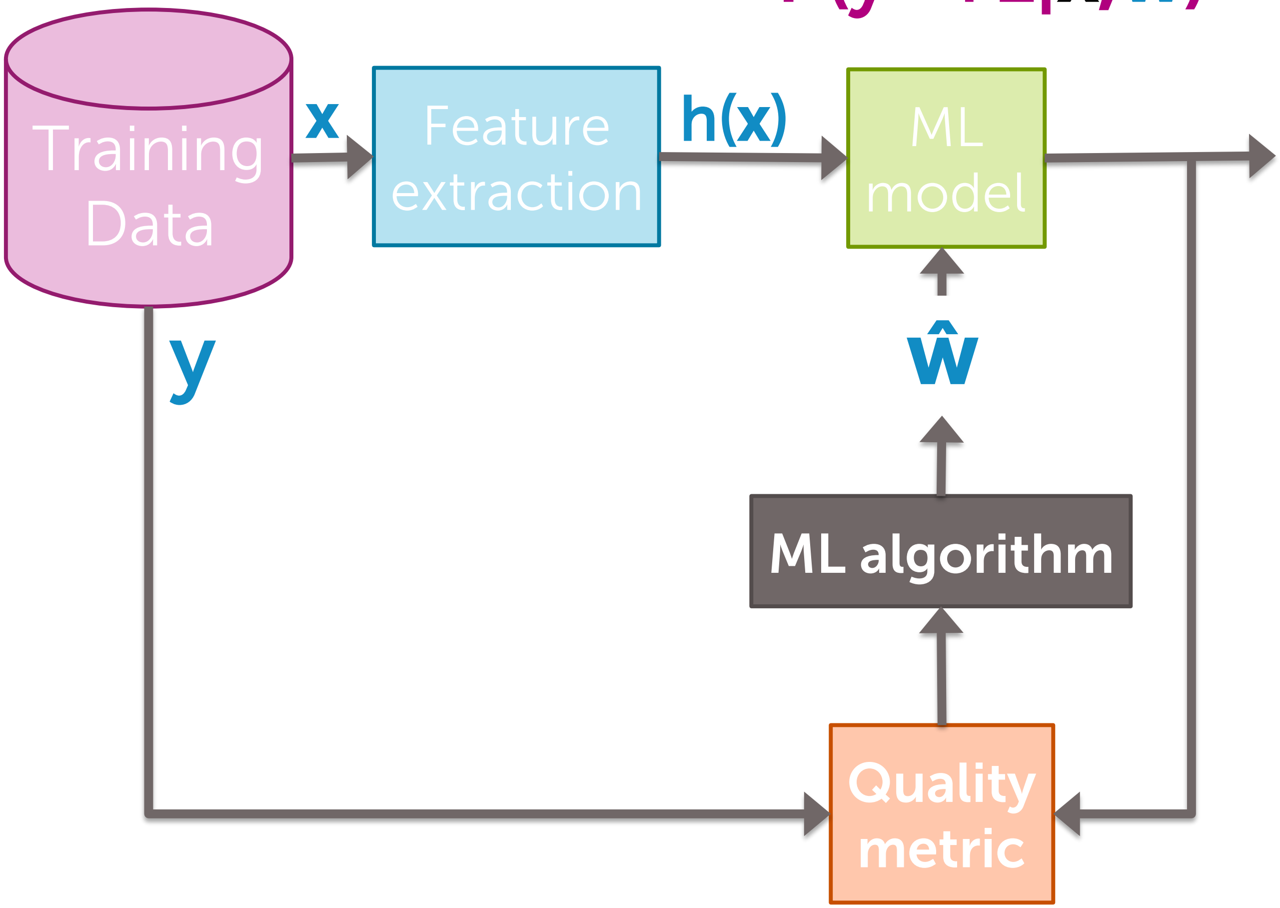
Regularization	λ = 0	λ = 0.00001	λ = 0.001	λ = 1
Range of coefficients	-3170 to 3803	-8.04 to 12.14	-0.70 to 1.25	-0.13 to 0.57
Learned probabilities				

highly over confident

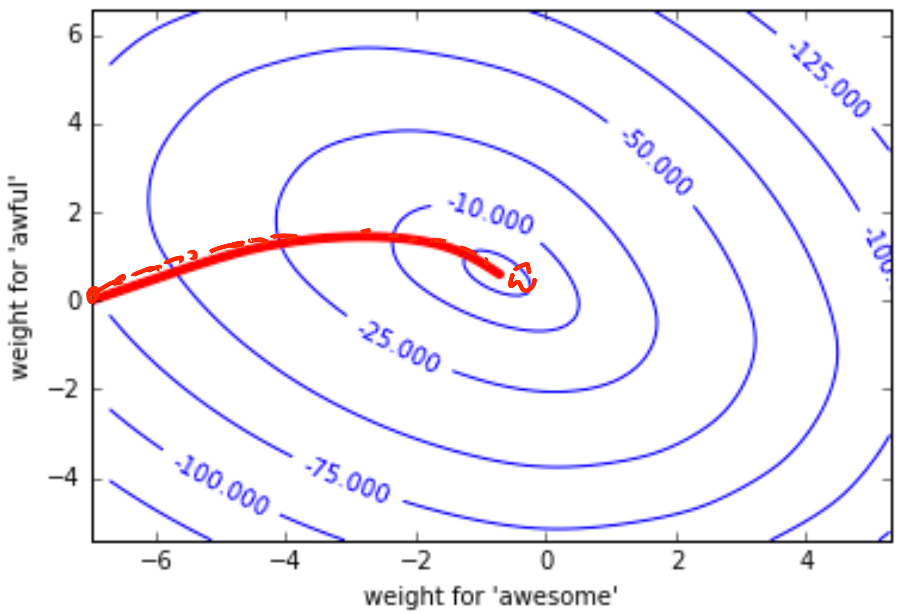
very natural uncertainty region

Finding best L_2 regularized linear classifier with gradient ascent

$$\hat{P}(y=+1|\mathbf{x},\hat{\mathbf{w}}) = \frac{1}{1+e^{-\hat{\mathbf{w}}^\top h(\mathbf{x})}}$$



Gradient ascent



Algorithm:

while not converged

$$\mathbf{w}^{(t+1)} \leftarrow \mathbf{w}^{(t)} + \eta \underbrace{\nabla \ell(\mathbf{w}^{(t)})}_{\text{need the gradient of regularized log likelihood}}$$

Gradient of L_2 regularized log-likelihood

Total quality =
measure of fit - measure of magnitude of coefficients

$$\underbrace{\text{measure of fit}}_{\ell(\mathbf{w})} - \underbrace{\text{measure of magnitude of coefficients}}_{\lambda \|\mathbf{w}\|_2^2}$$

$$\text{Total derivative} = \frac{\partial \ell(\mathbf{w})}{\partial \mathbf{w}_j} - \lambda \frac{\partial \|\mathbf{w}\|_2^2}{\partial \mathbf{w}_j}$$

Derivative of (log-)likelihood

Sum over data points

Feature value

Difference between truth and prediction

$$\frac{\partial \ell(\mathbf{w})}{\partial \mathbf{w}_j} = \sum_{i=1}^{N} h_j(\mathbf{x}_i)\underbrace{\Big(\mathbb{1}[y_i = +1] - P(y = +1 \mid \mathbf{x}_i, \mathbf{w})\Big)}_{\text{Difference between truth and prediction}}$$

Derivative of L_2 penalty

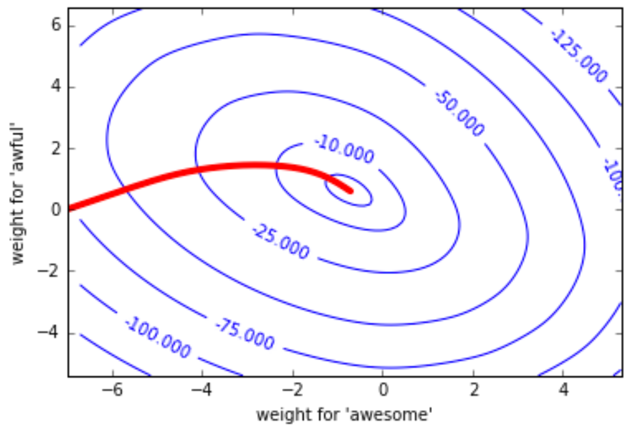
$$\frac{\partial ||\mathbf{w}||_2^2}{\partial \mathbf{w}_j} = \frac{\partial}{\partial w_j}\left[w_0^2 + w_1^2 + w_2^2 + \cdots + w_j^2 + \cdots + w_D^2\right] = 2w_j$$

Understanding contribution of L_2 regularization

$$\frac{\partial \ell(\mathbf{w})}{\partial \mathbf{w}_j} \overbrace{- 2\lambda \mathbf{w}_j}^{\text{Term from } L_2 \text{ penalty}}$$

	$-2\lambda w_j$	Impact on w_j
$w_j > 0$	< 0	decreases w_j $\Rightarrow$ w_j becomes closer to 0
$w_j < 0$	> 0	increases w_j $\Rightarrow$ w_j becomes closer to 0

Summary of gradient ascent for logistic regression with L_2 Regularization



init $\mathbf{w}^{(1)}$=0 (or randomly, or smartly), t=1

while not converged:

for j=0,…,D

partial[j] $= \sum_{i=1}^{N} h_j(\mathbf{x}_i)\Big(\mathbb{1}[y_i = +1] - P(y = +1 \mid \mathbf{x}_i, \mathbf{w}^{(t)})\Big)$

$\mathbf{w}_j^{(t+1)} \leftarrow \mathbf{w}_j^{(t)} + \eta\ (\text{partial[j]} - \underbrace{2\lambda\ \mathbf{w}_j^{(t)}}_{\text{only change !!}})$

t ← t + 1

step size

$\frac{\partial \ell(w)}{\partial w_j}$

Sparse logistic regression with L_1 regularization

Recall sparsity (many $\hat{\mathbf{w}}_j$=0) gives efficiency and interpretability

Efficiency:

- If size($\mathbf{w}$) = 100B, each prediction is expensive
- If $\hat{\mathbf{w}}$ sparse, computation only depends on # of non-zeros

many zeros

$$\hat{y}_i = sign\left(\sum_{\hat{\mathbf{w}}_j \neq 0} \hat{\mathbf{w}}_j h_j(\mathbf{x}_i)\right)$$

Interpretability:

- Which features are relevant for prediction?

Sparse logistic regression

Total quality =
$$\underbrace{\text{measure of fit}}_{\ell(\mathbf{w})} - \underbrace{\text{measure of magnitude of coefficients}}_{||\mathbf{w}||_1 = |w_0| + \ldots + |w_D|}$$

L_1 regularized logistic regression

Leads to **sparse** solutions!

L_1 regularized logistic regression

Just like L2 regularization, solution is governed by a continuous parameter λ

$$\ell(\mathbf{w}) - \lambda||\mathbf{w}||_1$$

tuning parameter = balance of fit and **sparsity**

If λ=0:

No regularization → standard MLE solution

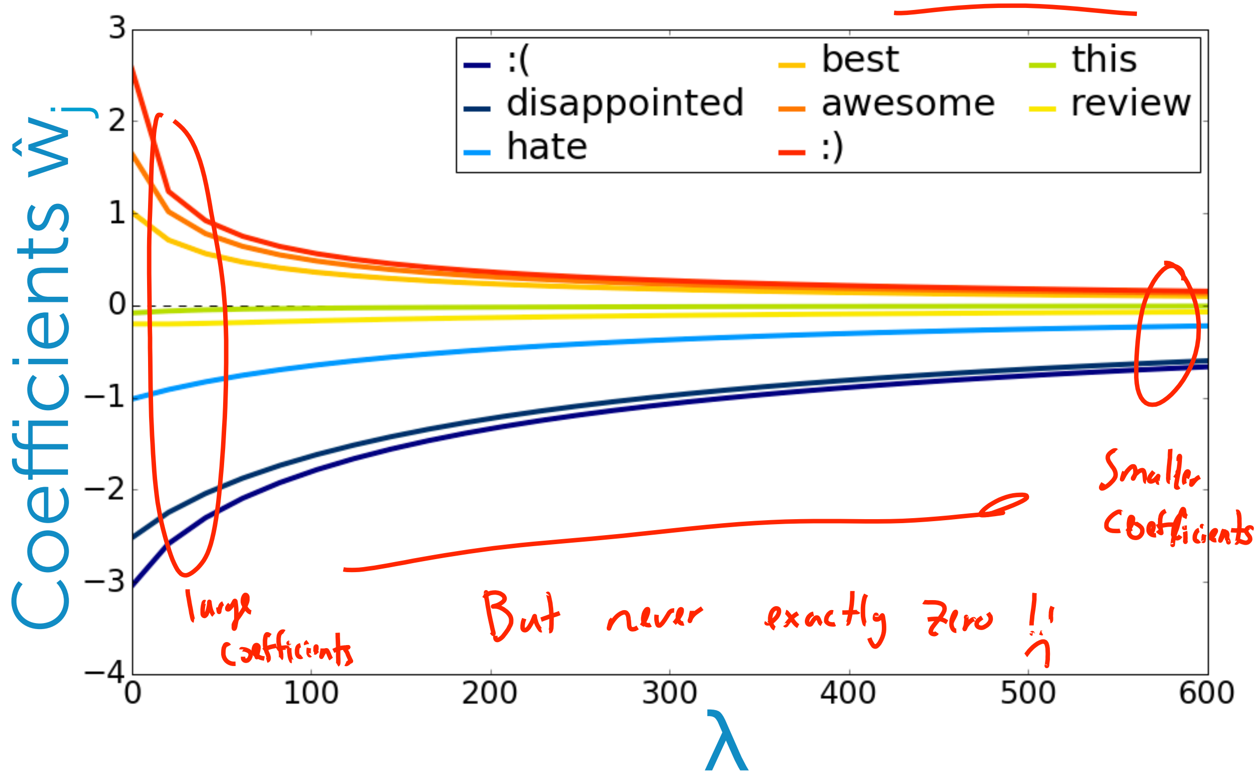
If $\lambda=\infty$:

all weight is on regularization → $\hat{w}=0$

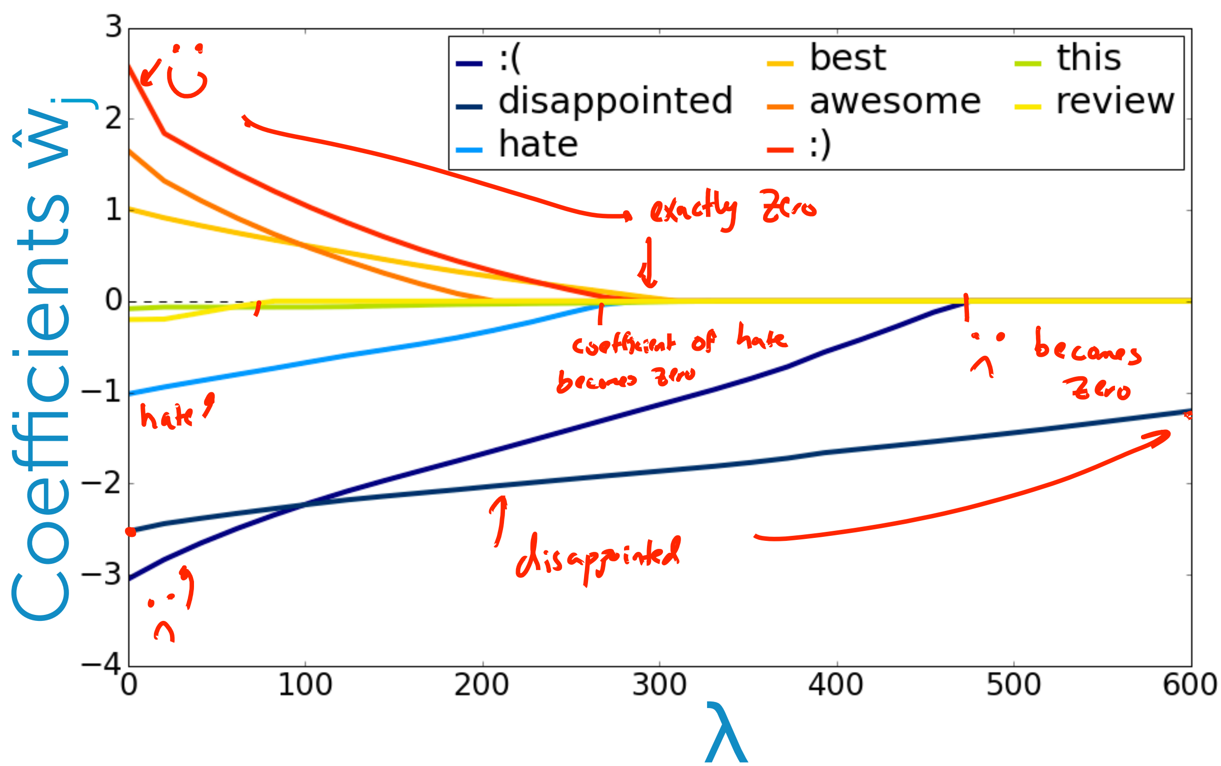
If λ in between:

Sparse solutions: some $\hat{w}_j \neq 0$, many other $\hat{w}_j = 0$

Regularization path – L_2 penalty



Regularization path – L_1 penalty



Summary of overfitting in logistic regression

What you can do now…

- Identify when overfitting is happening
- Relate large learned coefficients to overfitting
- Describe the impact of overfitting on decision boundaries and predicted probabilities of linear classifiers
- Motivate the form of L_2 regularized logistic regression quality metric
- Describe what happens to estimated coefficients as tuning parameter λ is varied
- Interpret coefficient path plot
- Estimate L_2 regularized logistic regression coefficients using gradient ascent
- Describe the use of L_1 regularization to obtain sparse logistic regression solutions