Regression and Classification

Samuel Cheng

School of ECE
University of Oklahoma

Spring, 2018

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Some notations and simple linear algebra

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A quick review of gradient

For a vector $\mathbf{x} = (x_1, x_2, \cdots, x_n)^T$, the gradient of a scalar multivariate function $f(\mathbf{x})$ is denoted by $\nabla f(\mathbf{x})$

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and $\nabla f(\mathbf{x})|_{(0,1,0)}$?

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$$\nabla f(\mathbf{x})|_{(0,1,0)} = (0, 0, 2)^T$$

Loss function for regression

Let us start with the regression problem. Recall from previously that

- We are trying to learn a function $f(x; W)$ such that for training input x_i and desired output y_i, $f(x_i; W) \sim y_i$

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- For regression, it is common to use mean square error for loss function, i.e., $l(f(x_i; W), y_i) = (f(x_i; W) - y_i)^2$

Linear regression

For example, try to predict the mass (weight) of a man based on his height, bmi, and his age (assuming we don't know what bmi is here)

- E.g., height = 1.8 m, bmi = 23, age =29, what is his mass?

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- Given training data, we need to find $\mathbf{w}$
  - $\mathbf{x}_1 = (1.68, 31.80, 43.34, 1)^T$, $y_1 = 87.50$
  - $\mathbf{x}_2 = (1.80, 33.11, 16.69, 1)^T$, $y_2 = 110.06$
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  - $\mathbf{x}_N = (1.83, 33.79, 43.30, 1)^T$, $y_N = 112.33$
- Write $X_{train} = \left(\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N\right)$ and $\mathbf{y}_{train} = (y_1, y_2, \cdots, y_N)^T$, we want

$$\mathbf{y}_{train} \sim X_{train}^T \mathbf{w}$$

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- MSE: 6.63. It is a bit high, let's try to reduce it

Expanding features...

- Let's include some higher "order" features. For the raw feature x_1, x_2, x_3, we can also include products of them as a feature. So a new feature vector becomes

$$(1, x_1, x_2, x_3, x_1^2, x_2^2, x_3^2, x_1x_2, x_1x_3, x_2x_3),$$

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- MSE: 1.01. Nice!

Expanding features (con't)...

- Let's go even higher order and also include products like $x_1 x_2 x_3$ and $x_1^2 x_2$. So the new feature vector now becomes

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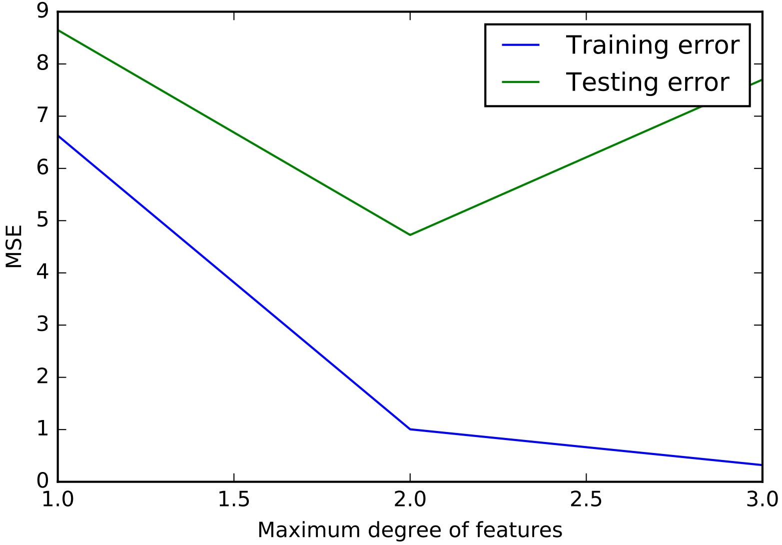
- Again we will do linear regression as before, the number of weights now increases from to 25
- MSE: 0.32...

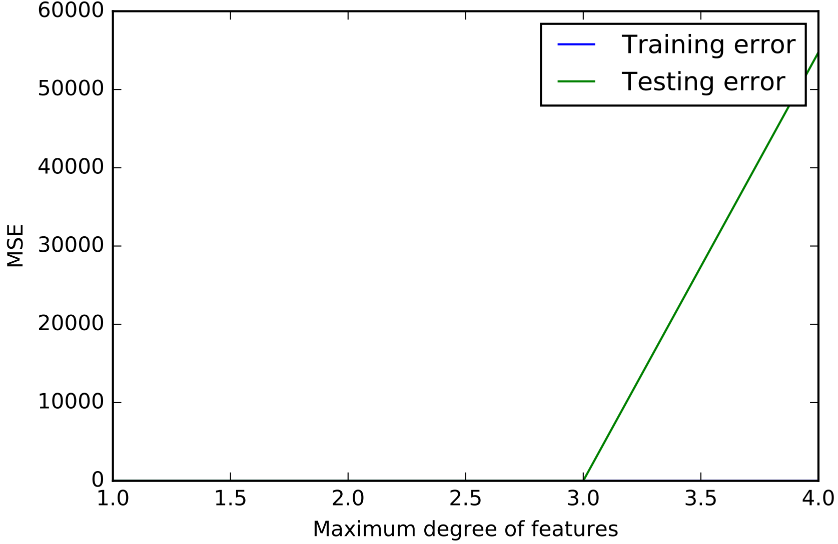
Expanding features (con't)...

- We can go further to the 4-th order and the number of weights now increases to 70
- MSE: 1.13e-12. Wow!

Wait, how about testing error?



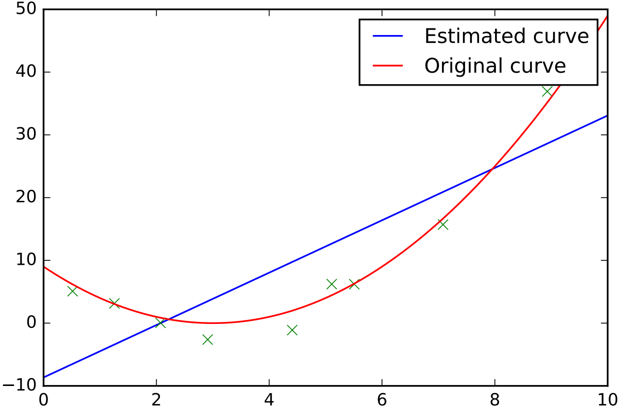
Wait, how about testing error...? Oops



Curve fitting

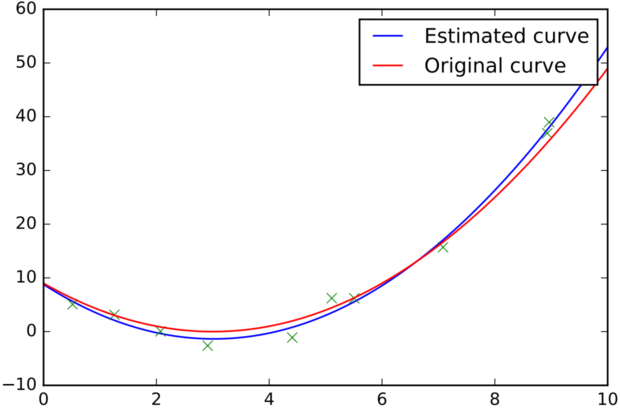
Why is it so bad for testing? Let's visit another even simpler example

- Let's try to fit a quadratic curve $y = (x-3)^2$ with linear regression. And again our training data will be wiggled a little bit by a Gaussian noise



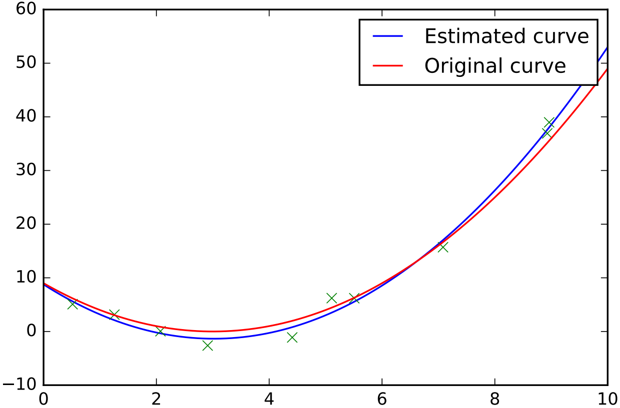
Curve fitting (2nd order)

Let's include higher order feature just as before. Take $(1, x, x^2)$ as feature by including x^2



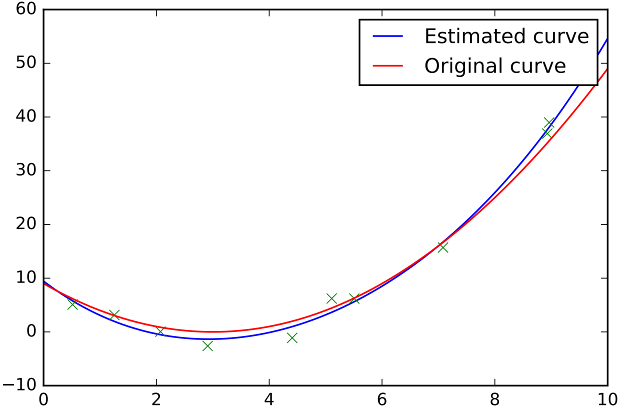
Curve fitting (3rd order)

$(1, x, x^2, x^3)$



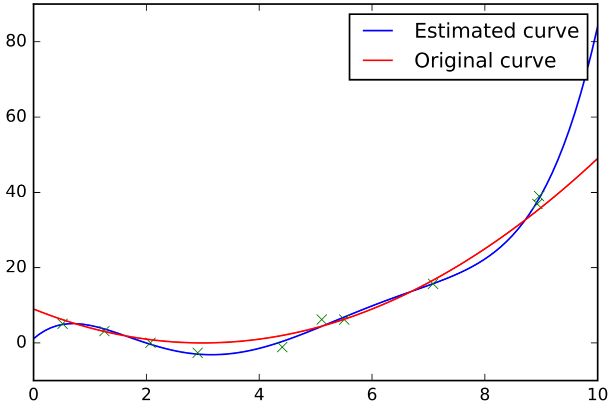
Curve fitting (4th order)

$(1, x, x^2, x^3, x^4)$



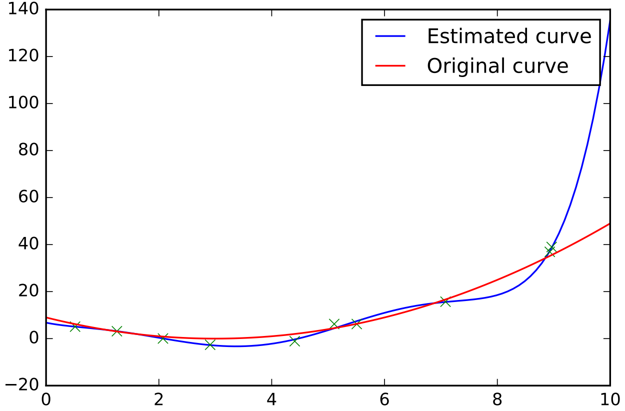
Curve fitting (5th order)

$(1, x, x^2, x^3, x^4, x^5)$



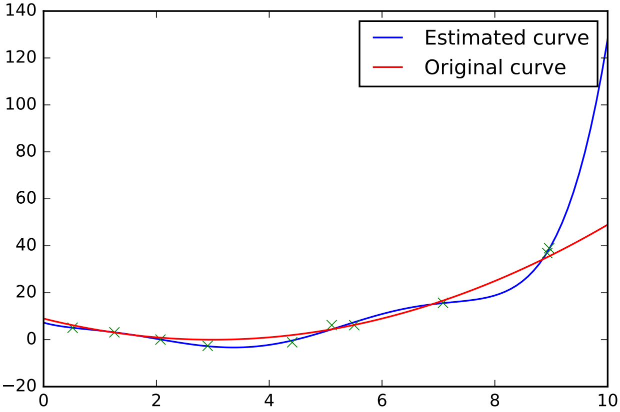
Curve fitting (6rd order)

$(1, x, x^2, x^3, x^4, x^5, x^6)$



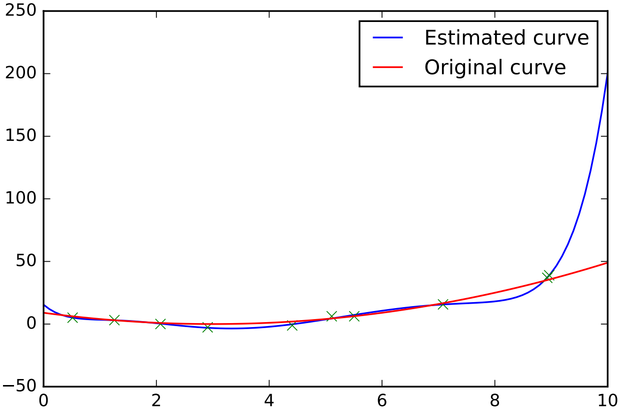
Curve fitting (7rd order)

$$(1, x, x^2, x^3, x^4, x^5, x^6, x^7)$$



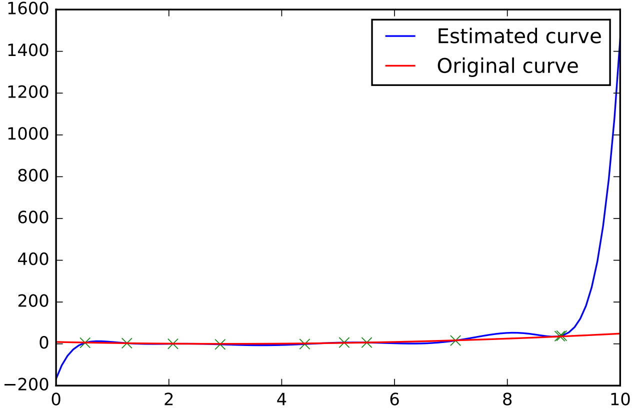
Curve fitting (8th order)

$(1, x, x^2, x^3, x^4, x^5, x^6, x^7, x^8)$

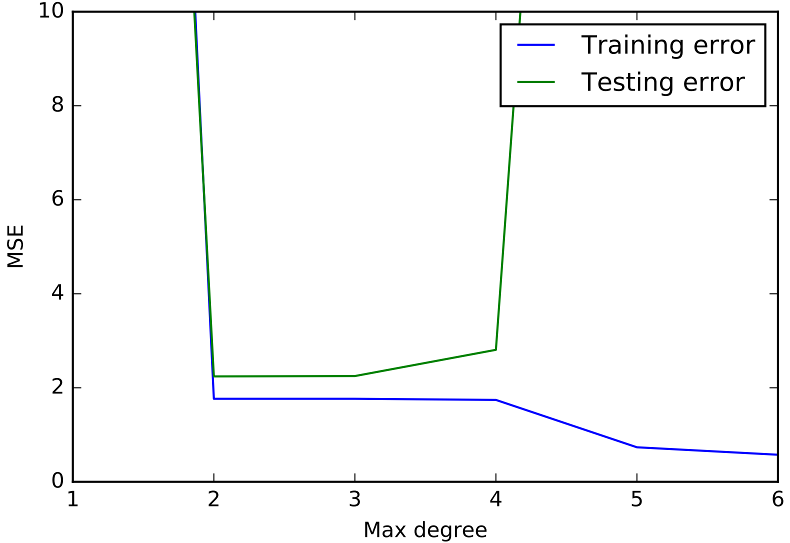


Curve fitting (9th order)

$$(1, x, x^2, x^3, x^4, x^5, x^6, x^7, x^8, x^9)$$



Overfitting vs underfitting



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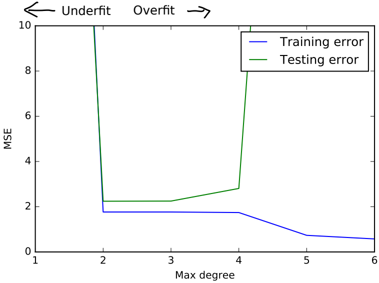
  - Unlike optimization, we don't actually know the true objective function
  - Loss function is just an approximated goal
- Should try to avoid neither overfitting nor underfitting
  - Everything should be made as simple as possible, but not simpler – Albert Einstein
  - Occam's razor: overly complex model is *not* a good thing (if you don't have sufficient data to fit the model)

High-bias vs high-variance

Sometimes we also refer to overfitting and underfitting roughly as high-variance and high-bias



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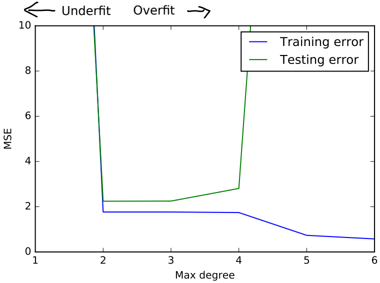
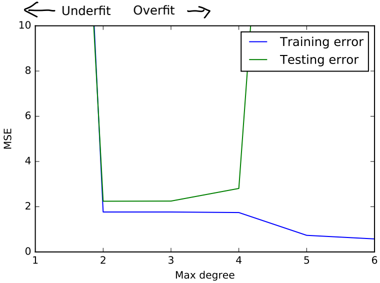
- High-bias: model is too rigid to learn (thus biased) and it cannot adapt to the data



High-bias vs high-variance

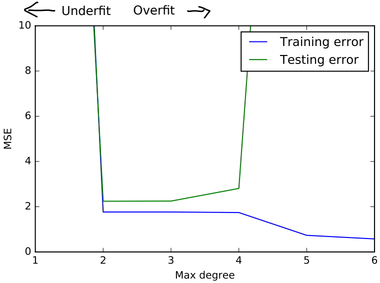
Sometimes we also refer to overfitting and underfitting roughly as high-variance and high-bias

- High-bias: model is too rigid to learn (thus biased) and it cannot adapt to the data
- High-variance: model is too elastic and can fit any arbitrary data. When fitted with different training data, the weights just converge to totally different values (thus high variance)



More on overfitting (high-variance)

- In the high-variance domain, the model is essentially learning the training data noise. That's why weights converge to different values for different training data
- Model complexity is relative. If more training data are available, the model used to be overfitted may not be overfitted anymore. So should we change a model every time we added new data?!



Regularization

Rather than using a simple model, we could restrain a more complex model from running wild with additional constraints. This process is commonly known as regularization

- As regularization can mitigate the overfitting problem, we can use a more expressive model even when we have only few data. And the same model can be used as data size increases
- A regularized complex model typically outperforms an unregularized simple model

Ridge regression

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$$= \frac{1}{2}\left(\mathbf{y}^T\mathbf{y} - \mathbf{w}^T X\mathbf{y} - \mathbf{y}^T X^T\mathbf{w} + \mathbf{w}[XX^T + \lambda I]\mathbf{w}\right)$$

- And the gradient is

$$\nabla_{\mathbf{w}} L(\mathbf{w}) = -X\mathbf{y} + [XX^T + \lambda I]\ \mathbf{w}$$

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- As before, if we set $\nabla_{\mathbf{w}} L(\mathbf{w}) = 0$, we have

$$\mathbf{w} = [XX^T + \lambda I]^{-1} X\mathbf{y}$$

Lasso

- Another common regularization is lasso. Instead of $\lambda \mathbf{w}^T \mathbf{w}$, the scaled l_1-norm of $\mathbf{w}$, $\lambda \|\mathbf{w}\|_1$ is added to the loss objective function Thus, we want to

$$\min_{\mathbf{w}} \frac{1}{2}(\mathbf{y} - X^T\mathbf{w})^T(\mathbf{y} - X^T\mathbf{w}) + \lambda \|\mathbf{w}\|_1,$$

where $\|\mathbf{w}\|_1 = |w_1| + |w_2| + \cdots + |w_D|$

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  - We will discuss how the optimization is typically performed later
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- Lasso tends to enforce a sparse weight solution. It was popular several years ago because of compressed sensing

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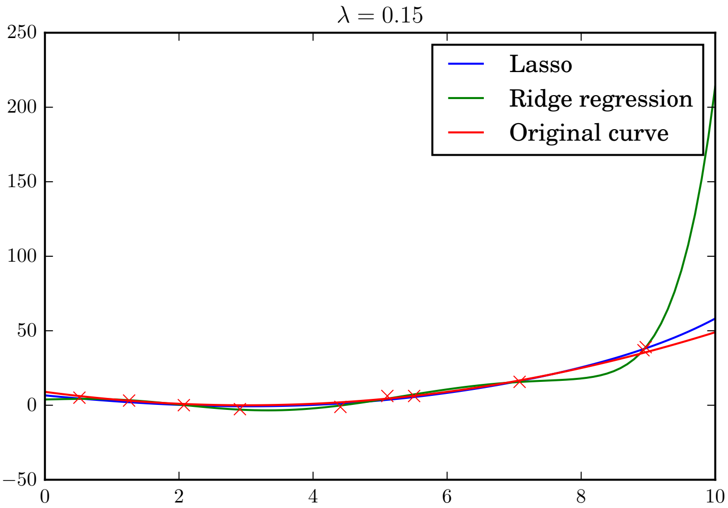
Curve fitting with Lasso and ridge regression (degree=9)



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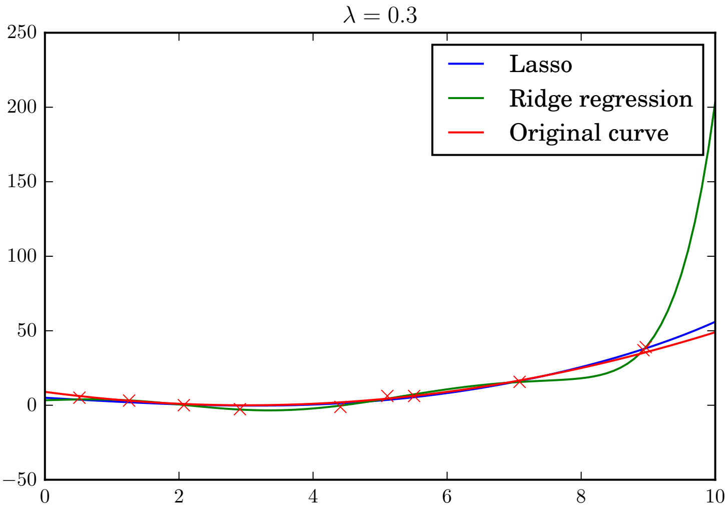

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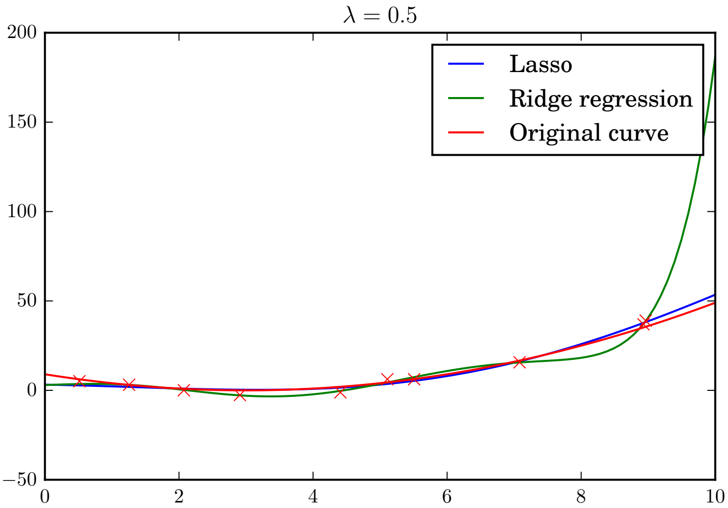

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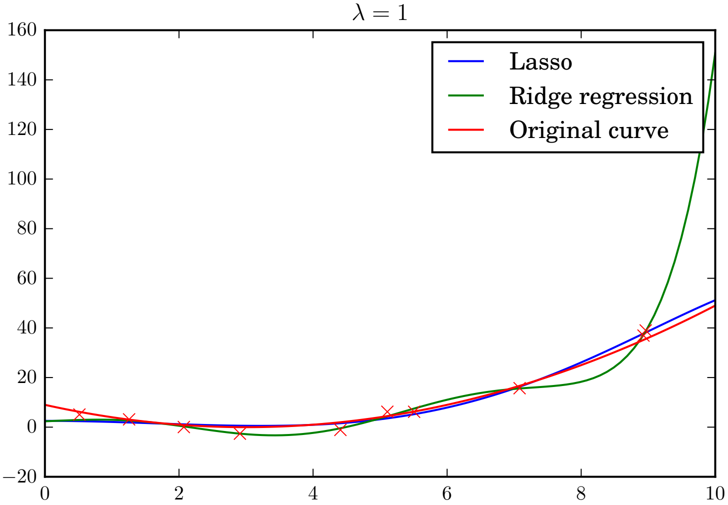

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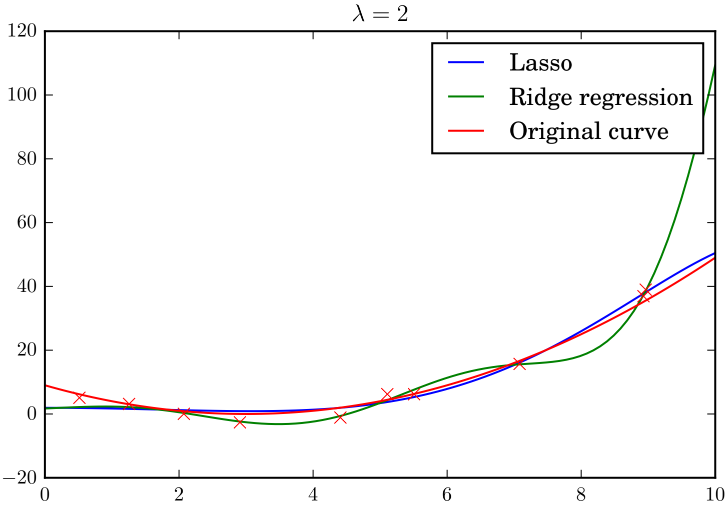

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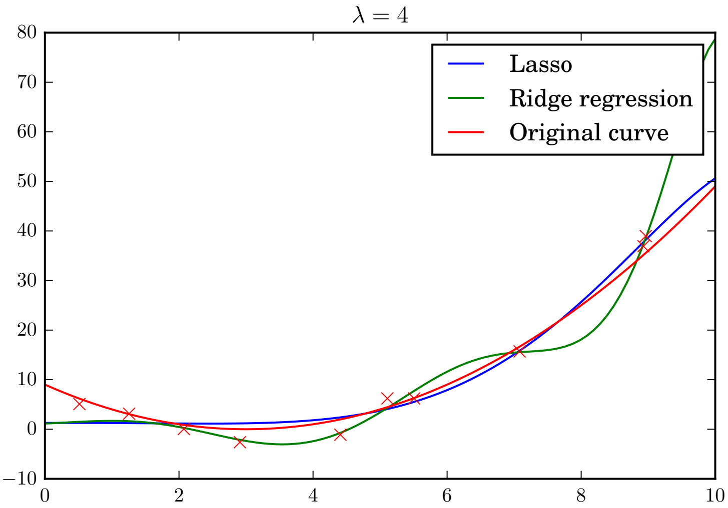

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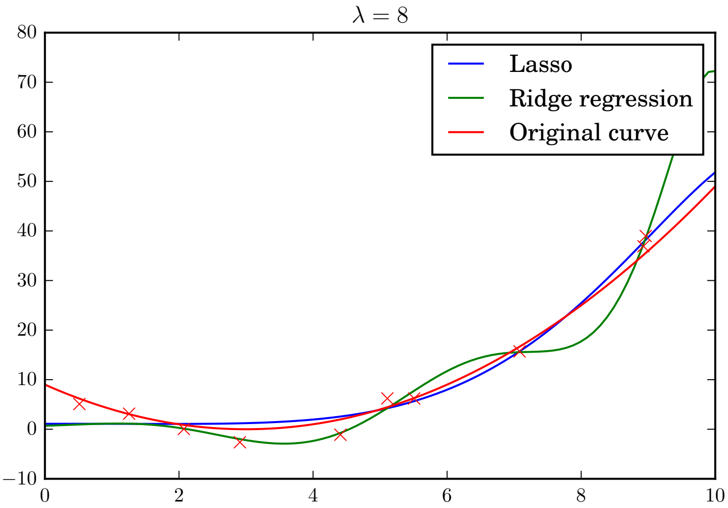

Conclusion

- Machine learning is all about generalization (from data)
- One can decrease the training error to arbitrarily small (by increasing model complexity)
- On the other hand, we really only care about test error, which is composed of
  - Bias: High bias when model is too rigid (model complexity is too low) to adapt to the training data
  - Variance: High variance when model is too flexible (model complexity is too high) that different sets of training data will converge to completely different weight parameters
- Occam's razor: a good explanation should be minimal

Conclusion

- For supervised learning systems (both classification and regression), we can typically reduce it to an optimization problem of minimizing a loss function (instead of training error) w.r.t. some weights
- Regularization terms can typically be incorporated in the loss function to keep the weights from running wild
- It is almost always better to use a more complex but regularized model than a simple model when one has sufficient training data
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  - That is why deep neural networks typically work better
    - Actually with sufficient data, we don't need to worry about overfitting
    - Furthermore, sometimes you may even want to overfit a small training set (attain 0 training error but large testing error) just to make sure your model is correct

Linear classification

The same linear regression idea can be transferred to classification problems

- Consider binary classification whether an image contains a cat or not
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  - We will decide if the image contains a cat of not by verifying if

$$\mathbf{x}^T \mathbf{w} \lessgtr 0,$$

where we will need to obtain the weight $\mathbf{w}$ through training (more later)

Logistic regression

- We can introduce a scoring function

$$f(\mathbf{x};\mathbf{w}) = H(\mathbf{x}^T\mathbf{w}),$$

where $H(t) = \begin{cases} 1, & t \geq 0 \\ 0, & t < 0 \end{cases}$ is a step function and we have a cat if $f(\mathbf{x};\mathbf{w}) = 1$ and no cat if $f(\mathbf{x};\mathbf{w}) = 0$

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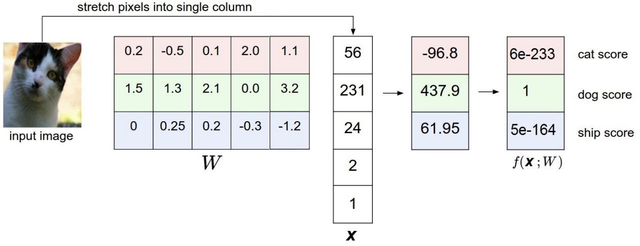
- Note that $f(\mathbf{x};\mathbf{w})$ essentially is a perceptron model and is difficult to train because of the discontinuity of $H(\cdot)$. Instead, we could replace $H(\cdot)$ by the sigmoid (or logistic) function $S(t) = \frac{1}{1+e^{-t}}$
  - Hence, known as logistic regression

Loss function of logistic regression

Another advantage of using $S(\cdot)$ is that we can interpret the output as probability and then the loss function can be specified by a "cross-entropy loss" as follows (will explain next)

$$L(\mathbf{w};\mathbf{x}) = \begin{cases} -\log f(\mathbf{x};\mathbf{w}), & \text{if the image is a cat} \\ -\log(1-f(\mathbf{x};\mathbf{w})), & \text{otherwise} \end{cases}$$

Softmax classifier



- For multiclass problem, we can extend the logistic scoring function to

$$f_i(\mathbf{x}; W) = \sigma_i(W\mathbf{x}),$$

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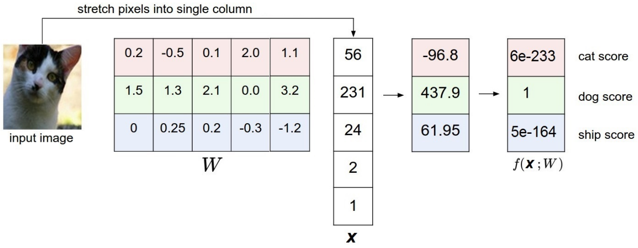

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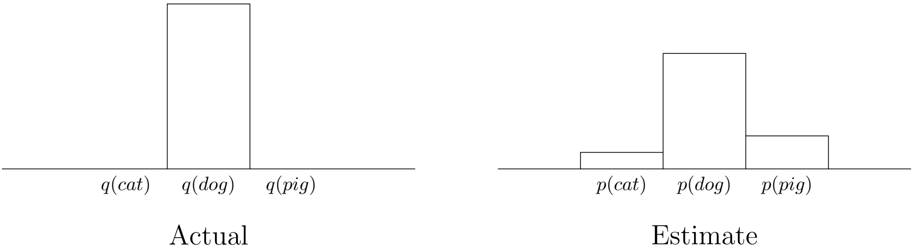
  where $\sigma_i(\mathbf{y}) = \frac{\exp(y_i)}{\sum_j \exp(y_j)}$ is known as a softmax function and is really just a normalized exponential function
- Again, we can interpret $f_i(\mathbf{x}; W)$ as the estimated probability of $\mathbf{x}$ belong to class i
  - E.g., $p(cat; \mathbf{x}, W) = f_{cat}(\mathbf{x}; W)$

Cross entropy loss function



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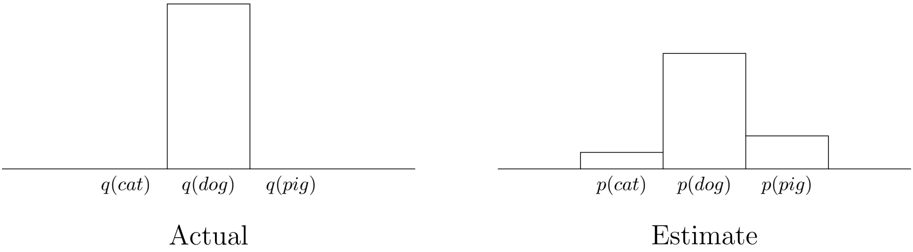

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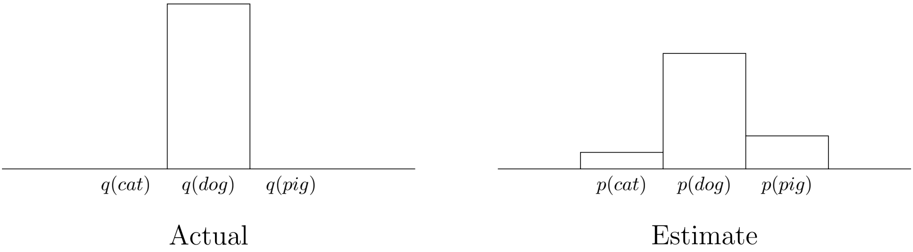

- Let say the image is actually a dog. We can express this as a distribution as shown on the left
- Ideally we would like the estimated probability distribution matches the actual one
- We can measure the difference between two distributions with KL-divergence given by

$$KL(q\|p) = \sum_i q_i \log \frac{q_i}{p_i}$$

KL-divergence is non-negative

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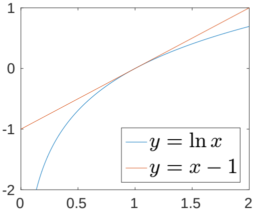

Fact

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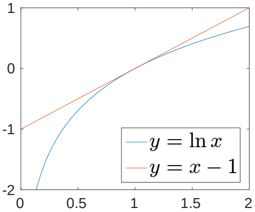

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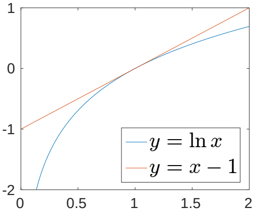

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Cross entropy loss function (con't)

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- The total loss is just sum over all training $\mathbf{x}$: $L(W) = \sum_{\mathbf{x}} L(W;\mathbf{x})$

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- So to optimize, we need to find the gradient of L wrt W

Derivative of softmax loss

- Recall that $L(W) = \sum_{\mathbf{x}} L(W; \mathbf{x}) = -\sum_{\mathbf{x}} \sum_l q_l^{(\mathbf{x})} \log \sigma_l(W\mathbf{x})$, where $q_j^{(\mathbf{x})}$ is non-zero $(= 1)$ only when j is the true label of $\mathbf{x}$

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- Write $L(W;\mathbf{x}) = \sum_l q_l \log \sigma_l(\mathbf{o})$, where $\mathbf{o} = W\mathbf{x}$. And we drop the superscript $(\mathbf{x})$ for clarity

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    - Recall that $L(W)$ supposes to a sum over individual loss of all training data $L(W;\mathbf{x})$
    - But $L(W)$ is really just an approximate as any training set is stochastic in natural in any case. Why not just approximate $L(W)$ not as refined with few data? That is, just pick a subset $\mathcal{X}_i$ from the training set and use

$$L_i(W) = \sum_{\mathbf{x}\in\mathcal{X}_i} L(W;\mathbf{x})$$

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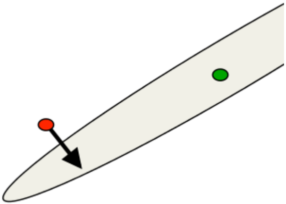
      instead. And this is known as the mini-batch gradient descent
- One may go to the extreme and only pick one $\mathbf{x}$ to estimate the gradient. This formally is known as the stochastic gradient descent. But in practice, no one uses it. But people often say stochastic gradient descent when they actually mean mini-batch gradient descent

Gradient descent with moment

- Going downhill reduces the error, but the direction of steepest descent does not point at the minimum unless the ellipse is a circle



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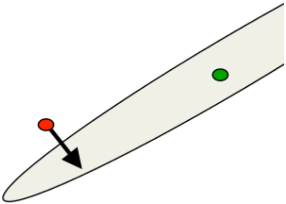

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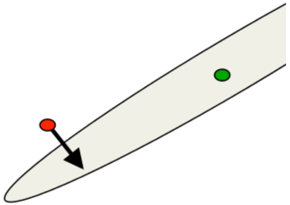
  - The gradient is small in the direction in which we want to travel a large distance
- A simple solution is to introduce "momentum" to the change of W. That is, $\Delta W = \lambda(\epsilon \nabla_W L(W)) + (1-\lambda)\Delta W^{(old)}$
- Will talk more about optimization methods later. So much for today



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- Actually, the numerical gradient is useful even if an analytical gradient exists. It at least provides a mean to debug your system
  - And luckily, for some packages such as Theano, they automatically find the analytical gradient for you

Conclusion

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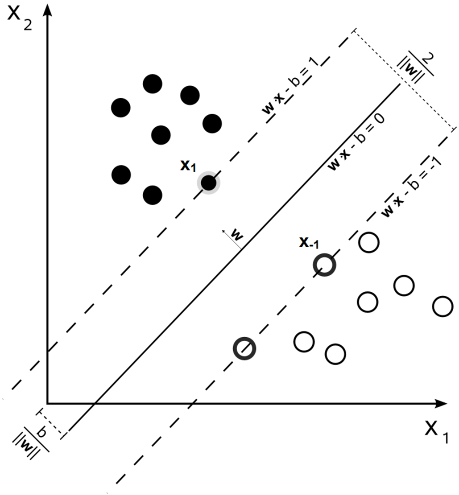
Conclusion

- For classification, we can feed the output of a linear regressor to a logistic function or softmax function to form a linear classifier
  - For only two classes, we have the logistic "regression" classifier
  - For multi-class cases, we have the softmax classifiers
- For finding the optimal weights, we may not be able to get the solution right away analytically (possible though for linear regression and ridge regression)
  - Can optimize iteratively with gradient descent
  - Can speed up gradient descent by using mini-batch instead of full batch
  - Momentum is a common trick to improve optimization efficiency also

SVM



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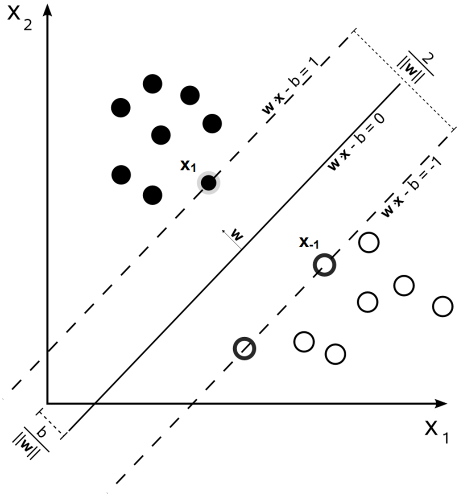

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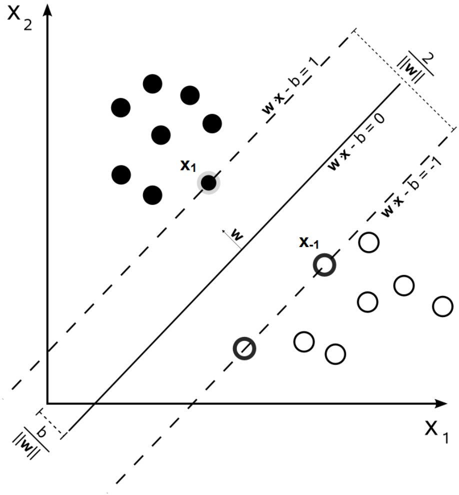

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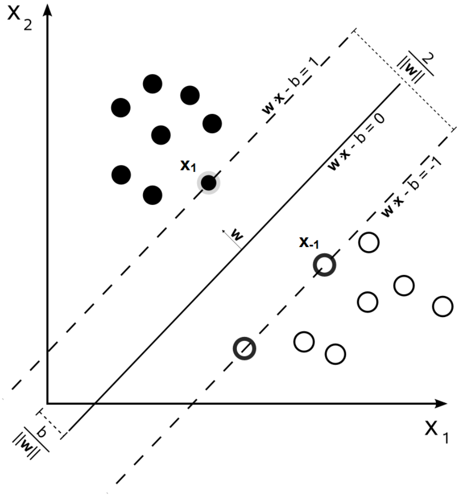

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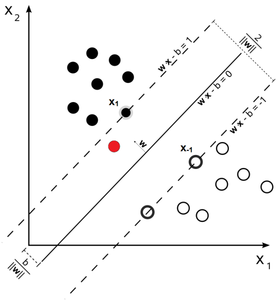
Equivalently,

$$\min \|\mathbf{w}\| \quad s.t. \quad y_i(\mathbf{w} \cdot \mathbf{x}_i - b) \geq 1$$

Soft-margin SVM and hinge loss



- Hard-margin SVM

$$\min \|\mathbf{w}\| \quad s.t. \quad y_i(\mathbf{w}\cdot\mathbf{x}_i - b) - 1 \geq 0$$

- Soft-margin SVM (allow constrain to be violate)
  - Define "hinge" loss function $h(z) = \max(0, z)$
  - Want to minimize hinge loss

$$\sum_i h(1 - y_i(\mathbf{w}\cdot\mathbf{x}_i - b))$$

  - Soft-margin SVM

$$\min \lambda\|\mathbf{w}\|^2 + \sum_i h(1 - y_i(\mathbf{w}\cdot\mathbf{x}_i - b))$$

Multi-class SVM

- We can easily extend soft-margin SVM to multi-class case. Let $s_l(\mathbf{x}) = \mathbf{w_l}^T \begin{bmatrix} 1 \\ \mathbf{x} \end{bmatrix}$ be the score for class l.

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Presentation logistics

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- Four bonus awards: (5% each) for the best presentation and (3% each) for first runner up according to my taste and popular votes from you all, respectively
- Tentatively reserve Tuesday classes for presentations

Software packages

	Pros	Cons
Caffe(2)	Don't need to write code	Adding module is harder (need C++); RNN is not support
(Py)Torch	Easy to create own module; Can do RNN	Lua (check out PyTorch)
Theano	Flexible and powerful	Kind of low-level
Tensorflow	Industry loves it. Most popular	Slow
Keras / Lasagne	Less verbose than Theano	Less flexible
MXnet	Rumored to be fast	Unpopular
Matconvnet	MATLAB	CNN only
CNTK (MS)	?	?
Paddle (Baidu)	?	?

Watch this CS231n lecture

Final reminder

Assignment 1 and package selection will be due **next Thursday**