CS490 Lecture 2: Linear Regression

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Adapted from Roger Grosse

Overview

- First learning algorithm of the course: linear regression
  - Task: predict scalar-valued targets, e.g. stock prices (hence "regression")
  - Architecture: linear function of the inputs (hence "linear")

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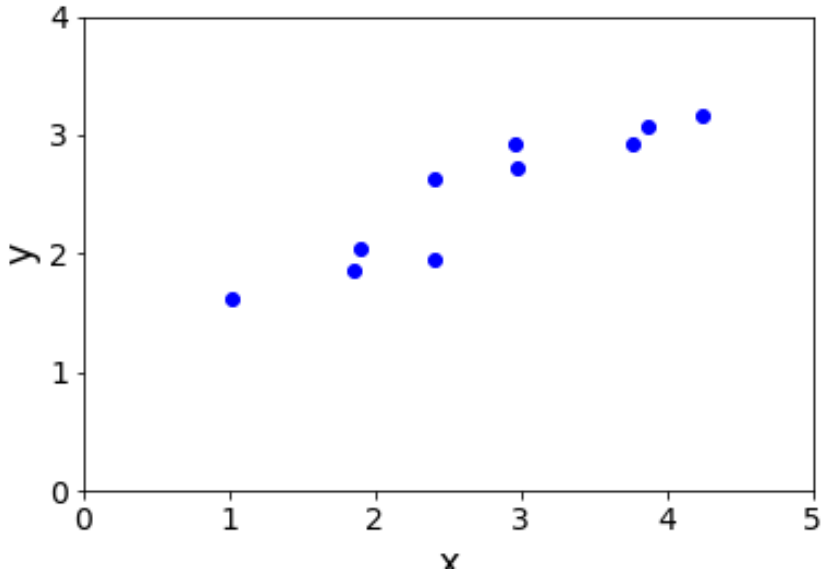
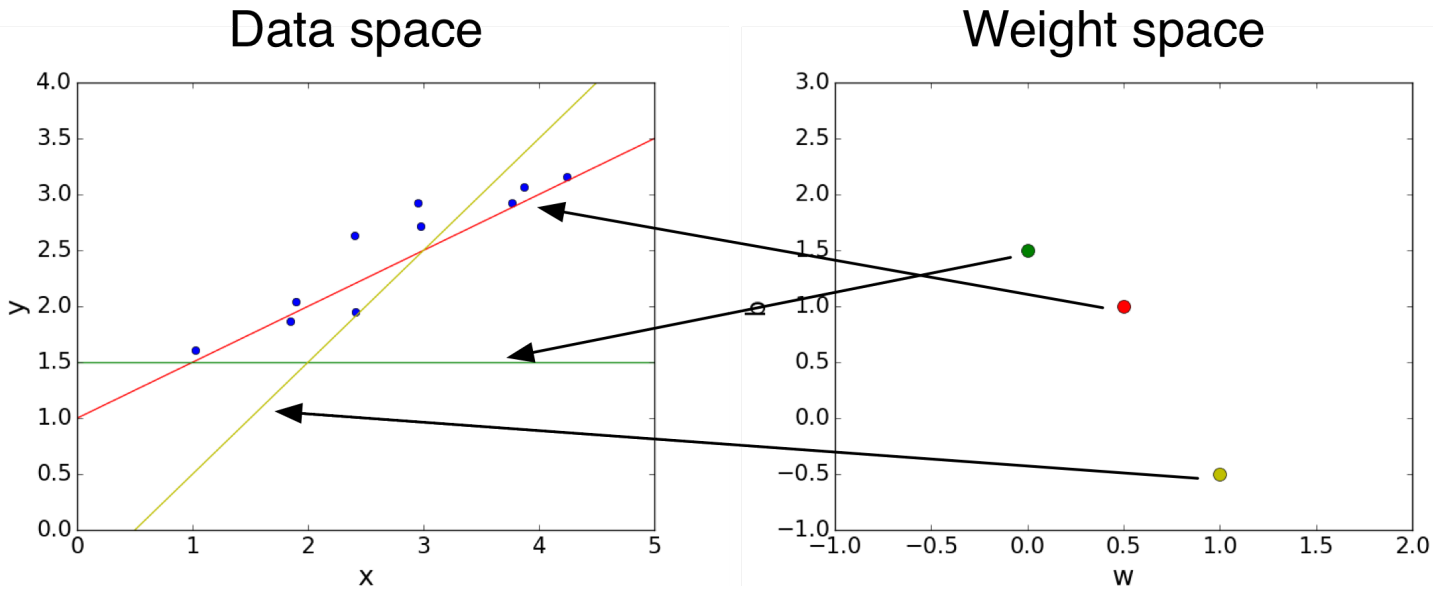
- First learning algorithm of the course: linear regression
  - Task: predict scalar-valued targets, e.g. stock prices (hence "regression")
  - Architecture: linear function of the inputs (hence "linear")
- Example of recurring themes throughout the course:
  - choose an architecture and a loss function
  - formulate an optimization problem
  - solve the optimization problem using one of two strategies
    - direct solution (set derivatives to zero)
    - gradient descent
  - vectorize the algorithm, i.e. represent in terms of linear algebra
  - make a linear model more powerful using features
  - understand how well the model generalizes

Problem Setup



- Want to predict a scalar t as a function of a scalar x
- Given a dataset of pairs $\{(\mathbf{x}^{(i)}, t^{(i)})\}_{i=1}^{N}$
- The $\mathbf{x}^{(i)}$ are called inputs, and the $t^{(i)}$ are called targets.

Problem Setup

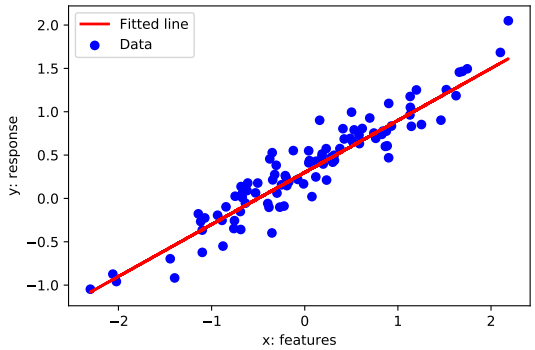


- **Model:** y is a linear function of x:

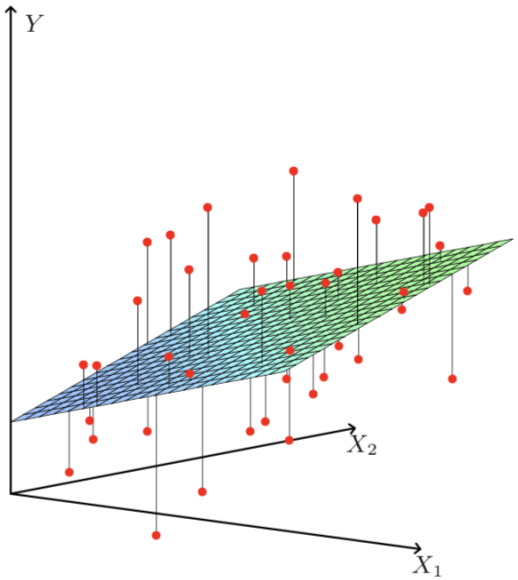
$$y = wx + b$$

- y is the prediction
- w is the weight
- b is the bias
- w and b together are the parameters
- Settings of the parameters are called hypotheses

What is Linear? 1 feature vs D features



- If we have only 1 feature:
  $y = wx + b$ where $w, x, b \in \mathbb{R}$.
- y is linear in x.



- If we have D features:
  $y = \mathbf{w}^\top \mathbf{x} + b$ where $\mathbf{w}, \mathbf{x} \in \mathbb{R}^D$,
  $b \in \mathbb{R}$
- y is linear in $\mathbf{x}$.

Relation between the prediction y and inputs $\mathbf{x}$ is linear in both cases.

Problem Setup

- **Loss function:** squared error

$$\mathcal{L}(y, t) = \frac{1}{2}(y - t)^2$$

- $y - t$ is the residual, and we want to make this small in magnitude
- The $\frac{1}{2}$ factor is just to make the calculations convenient.

Problem Setup

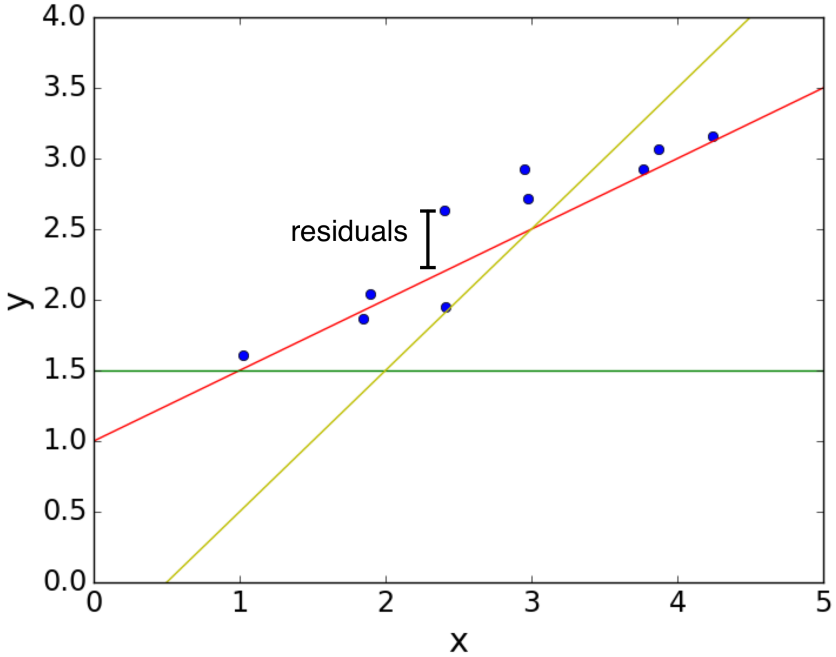
- **Loss function:** squared error

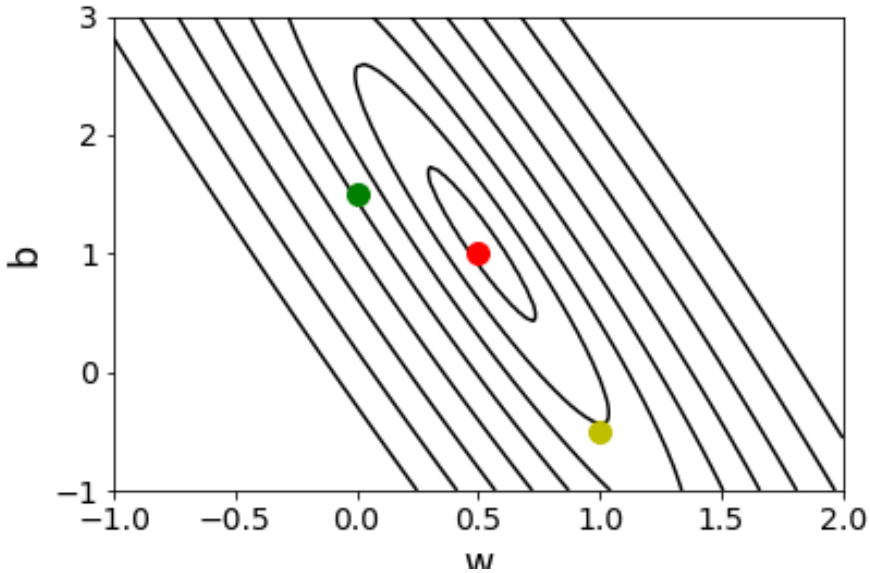
$$\mathcal{L}(y, t) = \frac{1}{2}(y - t)^2$$

- $y - t$ is the residual, and we want to make this small in magnitude
- The $\frac{1}{2}$ factor is just to make the calculations convenient.
- **Cost function:** loss function averaged over all training examples

$$\begin{aligned}\mathcal{E}(w, b) &= \frac{1}{2N} \sum_{i=1}^{N} \left(y^{(i)} - t^{(i)} \right)^2 \\ &= \frac{1}{2N} \sum_{i=1}^{N} \left(wx^{(i)} + b - t^{(i)} \right)^2\end{aligned}$$

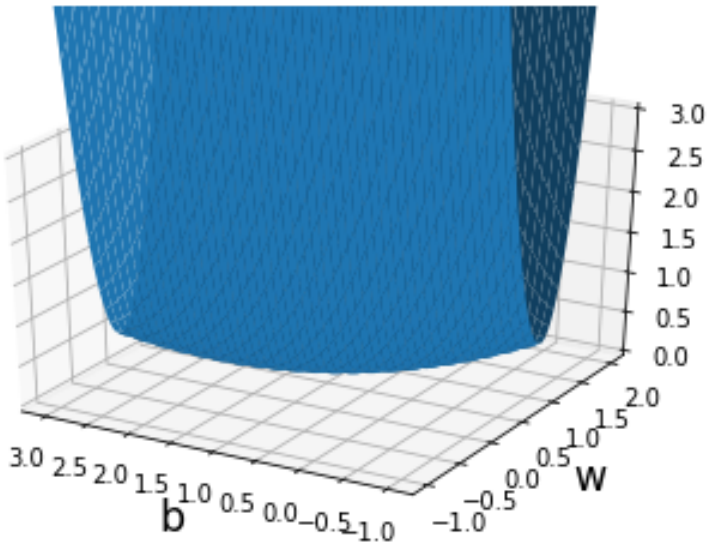
Problem Setup

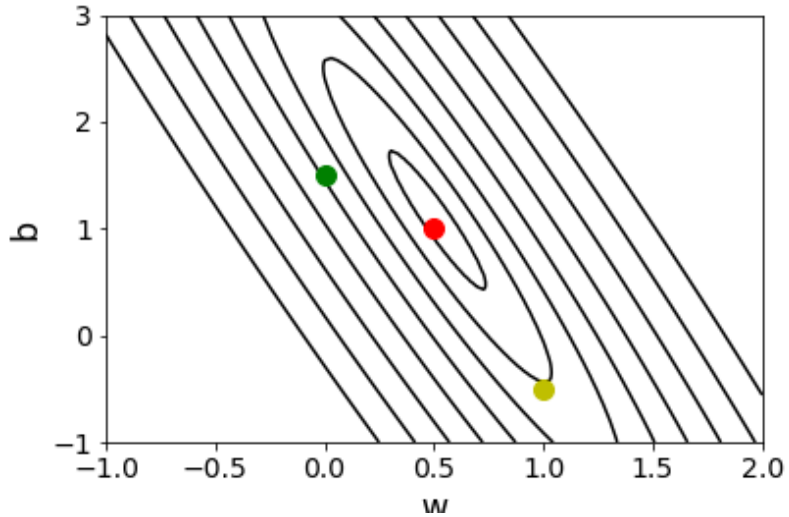




Problem Setup

Surface plot vs. contour plot





Problem setup

- Suppose we have multiple inputs $x_1, \ldots, x_D$. This is referred to as multivariable regression.
- This is no different than the single input case, just harder to visualize.
- Linear model:

$$y = \sum_j w_j x_j + b$$

Vectorization

- Computing the prediction using a for loop:

```
y = b
for j in range(M):
    y += w[j] * x[j]
```

- For-loops in Python are slow, so we vectorize algorithms by expressing them in terms of vectors and matrices.

$$\mathbf{w} = (w_1, \ldots, w_D)^\top \qquad \mathbf{x} = (x_1, \ldots, x_D)$$

$$y = \mathbf{w}^\top \mathbf{x} + b$$

- This is simpler and much faster:

```
y = np.dot(w, x) + b
```

Vectorization

Why vectorize?

Vectorization

Why vectorize?

- The equations, and the code, will be simpler and more readable. Gets rid of dummy variables/indices!
- Vectorized code is much faster
  - Cut down on Python interpreter overhead
  - Use highly optimized linear algebra libraries
  - Matrix multiplication is very fast on a Graphics Processing Unit (GPU)

Vectorization

- We can take this a step further. Organize all the training examples into a matrix $\mathbf{X}$ with one row per training example, and all the targets into a vector $\mathbf{t}$.

one feature across all training examples

$$\mathbf{X} = \begin{pmatrix} \mathbf{x}^{(1)\top} \\ \mathbf{x}^{(2)\top} \\ \mathbf{x}^{(3)\top} \end{pmatrix} = \begin{pmatrix} 8 & 0 & 3 & 0 \\ 6 & -1 & 5 & 3 \\ 2 & 5 & -2 & 8 \end{pmatrix}$$

one training example (vector)

- Computing the predictions for the whole dataset:

$$\mathbf{X}\mathbf{w} + b\mathbf{1} = \begin{pmatrix} \mathbf{w}^\top \mathbf{x}^{(1)} + b \\ \vdots \\ \mathbf{w}^\top \mathbf{x}^{(N)} + b \end{pmatrix} = \begin{pmatrix} y^{(1)} \\ \vdots \\ y^{(N)} \end{pmatrix} = \mathbf{y}$$

Vectorization

- Computing the squared error cost across the whole dataset:

$$\mathbf{y} = \mathbf{X}\mathbf{w} + b\mathbf{1}$$

$$\mathcal{E} = \frac{1}{2N}\|\mathbf{y} - \mathbf{t}\|^2$$

- In Python:

```
y = np.dot(X, w) + b
cost = np.sum((y - t) ** 2) / (2. * N)
```

- **Example in tutorial**

Solving the optimization problem

- We defined a cost function. This is what we'd like to minimize.
- Recall from calculus class: minimum of a smooth function (if it exists) occurs at a critical point, i.e. point where the derivative is zero.
- Multivariate generalization: set the partial derivatives to zero. We call this direct solution.

Direct solution

- Partial derivatives: derivatives of a multivariate function with respect to one of its arguments.

$$\frac{\partial}{\partial x_1} f(x_1, x_2) = \lim_{h \to 0} \frac{f(x_1 + h, x_2) - f(x_1, x_2)}{h}$$

- To compute, take the single variable derivatives, pretending the other arguments are constant.
- Example: partial derivatives of the prediction y

$$\begin{aligned}
\frac{\partial y}{\partial w_j} &= \frac{\partial}{\partial w_j} \left[\sum_{j'} w_{j'} x_{j'} + b \right] \\
&= x_j \\
\frac{\partial y}{\partial b} &= \frac{\partial}{\partial b} \left[\sum_{j'} w_{j'} x_{j'} + b \right] \\
&= 1
\end{aligned}$$

Direct solution

- Chain rule for derivatives:

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial w_j} &= \frac{\mathrm{d}\mathcal{L}}{\mathrm{d}y}\frac{\partial y}{\partial w_j} \\ &= \frac{\mathrm{d}}{\mathrm{d}y}\left[\frac{1}{2}(y-t)^2\right] \cdot x_j \\ &= (y-t)x_j \\ \frac{\partial \mathcal{L}}{\partial b} &= y - t\end{aligned}$$

- We will give a more precise statement of the Chain Rule in a few weeks. It's actually pretty complicated.
- Cost derivatives (average over data points):

$$\begin{aligned}\frac{\partial \mathcal{E}}{\partial w_j} &= \frac{1}{N}\sum_{i=1}^{N}(y^{(i)} - t^{(i)})\, x_j^{(i)} \\ \frac{\partial \mathcal{E}}{\partial b} &= \frac{1}{N}\sum_{i=1}^{N} y^{(i)} - t^{(i)}\end{aligned}$$

Direct solution

- The minimum must occur at a point where the partial derivatives are zero.

$$\frac{\partial \mathcal{E}}{\partial w_j} = 0 \qquad \frac{\partial \mathcal{E}}{\partial b} = 0.$$

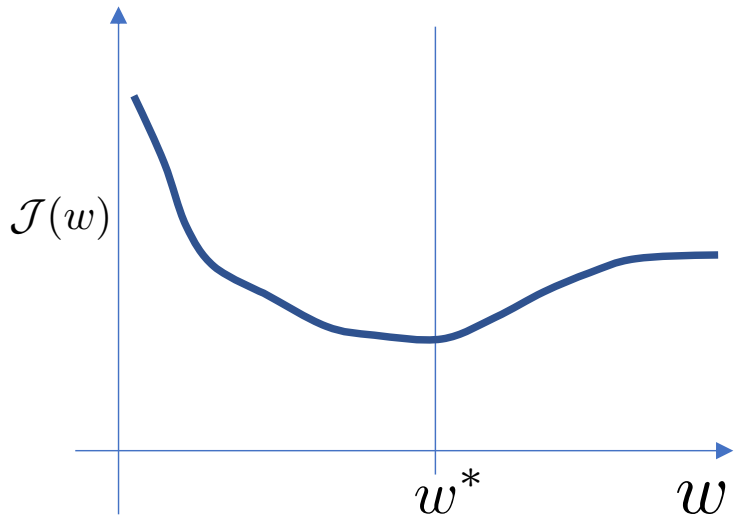
- If $\partial \mathcal{E}/\partial w_j \neq 0$, you could reduce the cost by changing w_j.
- This turns out to give a system of linear equations, which we can solve efficiently. **Full derivation in tutorial and the readings.**
- Optimal weights:

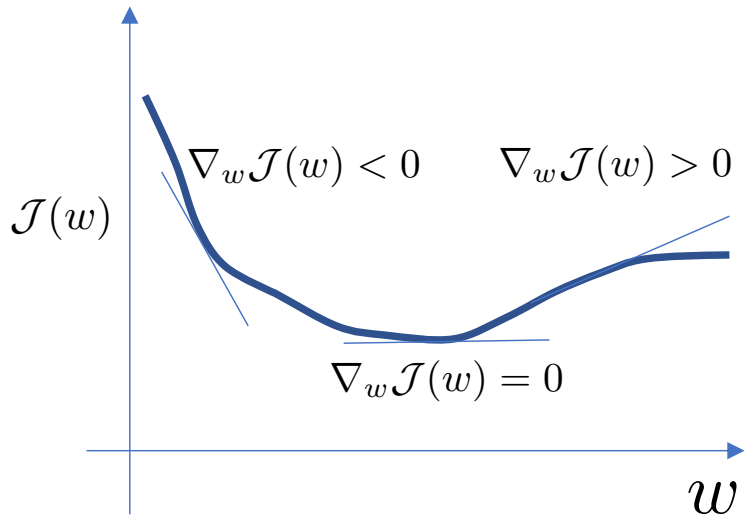
$$\mathbf{w} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{t}$$

- Linear regression is one of only a handful of models in this course that permit direct solution.

Direct Solution: Calculus

- Lets consider a cartoon visualization of $\mathcal{J}(w)$ where w is single dimensional
- **Left** We seek $w = w^*$ that minimizes $\mathcal{J}(w)$
- **Right** The gradients of a function can tell us where the maxima and minima of functions lie
- **Strategy:** Write down an algebraic expression for $\nabla_w \mathcal{J}(w)$. Set equation to 0. Solve for w





Gradient Descent

- Now let's see a second way to minimize the cost function which is more broadly applicable: gradient descent.
- Gradient descent is an iterative algorithm, which means we apply an update repeatedly until some criterion is met.
- We initialize the weights to something reasonable (e.g. all zeros) and repeatedly adjust them in the direction of steepest descent.

Iterative solution: Gradient Descent

- Most optimization problems we cover in this course don't have a direct solution.
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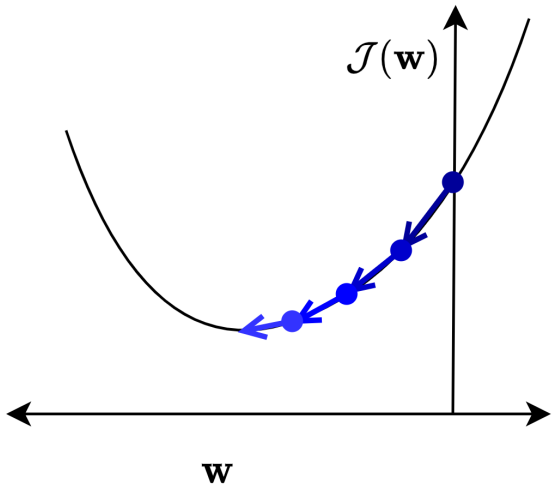
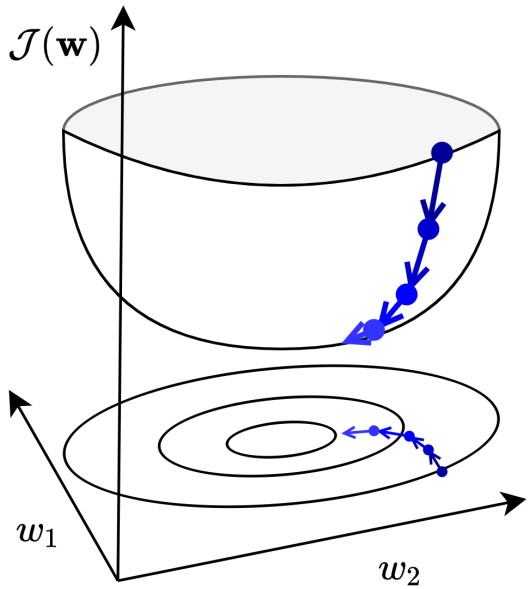




Gradient descent

- Observe:
  - if $\partial \mathcal{E}/\partial w_j > 0$, then increasing w_j increases $\mathcal{E}$.
  - if $\partial \mathcal{E}/\partial w_j < 0$, then increasing w_j decreases $\mathcal{E}$.
- The following update decreases the cost function:

$$w_j \leftarrow w_j - \alpha \frac{\partial \mathcal{E}}{\partial w_j}$$

$$= w_j - \frac{\alpha}{N} \sum_{i=1}^{N} (y^{(i)} - t^{(i)})\, x_j^{(i)}$$

- α is a learning rate. The larger it is, the faster $\mathbf{w}$ changes.
  - We'll see later how to tune the learning rate, but values are typically small, e.g. 0.01 or 0.0001

Gradient descent

- This gets its name from the gradient:

$$\frac{\partial \mathcal{E}}{\partial \mathbf{w}} = \begin{pmatrix} \frac{\partial \mathcal{E}}{\partial w_1} \\ \vdots \\ \frac{\partial \mathcal{E}}{\partial w_D} \end{pmatrix}$$

  - This is the direction of fastest increase in $\mathcal{E}$.

Gradient descent

- This gets its name from the gradient:

$$\frac{\partial \mathcal{E}}{\partial \mathbf{w}} = \begin{pmatrix} \frac{\partial \mathcal{E}}{\partial w_1} \\ \vdots \\ \frac{\partial \mathcal{E}}{\partial w_D} \end{pmatrix}$$

  - This is the direction of fastest increase in $\mathcal{E}$.
- Update rule in vector form:

$$\begin{aligned} \mathbf{w} &\leftarrow \mathbf{w} - \alpha \frac{\partial \mathcal{E}}{\partial \mathbf{w}} \\ &= \mathbf{w} - \frac{\alpha}{N} \sum_{i=1}^{N} (y^{(i)} - t^{(i)}) \, \mathbf{x}^{(i)} \end{aligned}$$

- Hence, gradient descent updates the weights in the direction of fastest *decrease*.

Gradient descent

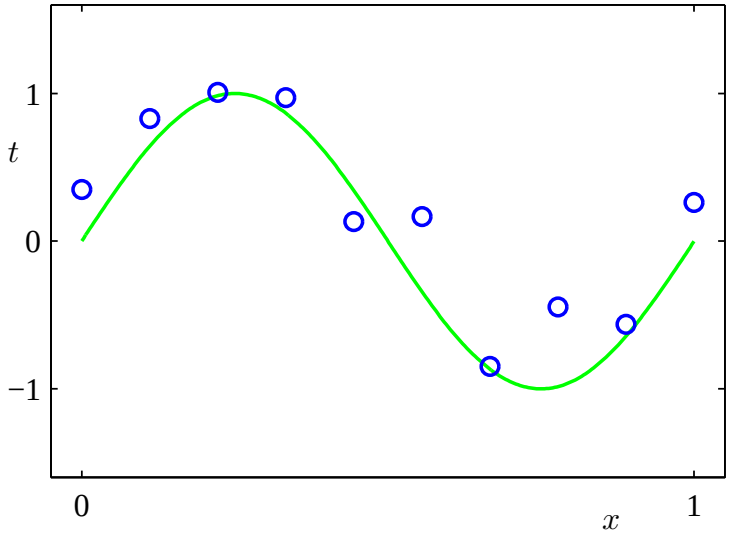
Visualization:
http://www.cs.toronto.edu/~guerzhoy/321/lec/W01/linear_regression.pdf#page=21

Gradient descent

- Why gradient descent, if we can find the optimum directly?
  - GD can be applied to a much broader set of models
  - GD can be easier to implement than direct solutions, especially with automatic differentiation software
  - For regression in high-dimensional spaces, GD is more efficient than direct solution (matrix inversion is an $\mathcal{O}(D^3)$ algorithm).

Feature mappings

- Suppose we want to model the following data



-Pattern Recognition and Machine Learning, Christopher Bishop.

- One option: fit a low-degree polynomial; this is known as polynomial regression

$$y = w_3 x^3 + w_2 x^2 + w_1 x + w_0$$

- Do we need to derive a whole new algorithm?

Feature mappings

- We get polynomial regression for free!
- Define the feature map

$$\phi(x) = \begin{pmatrix} 1 \\ x \\ x^2 \\ x^3 \end{pmatrix}$$

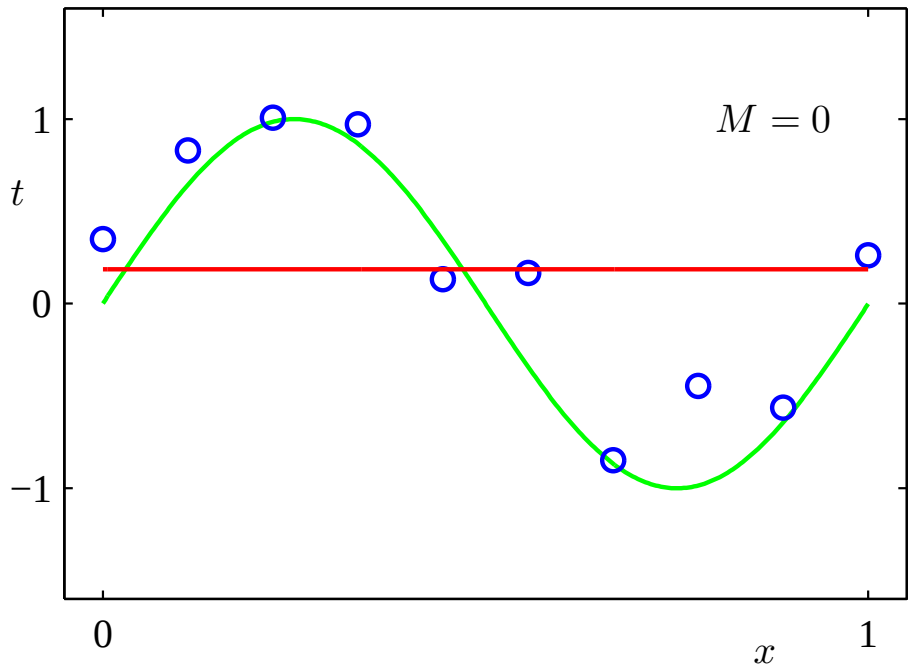
- Polynomial regression model:

$$y = \mathbf{w}^\top \phi(x)$$

- All of the derivations and algorithms so far in this lecture remain exactly the same!

Fitting polynomials

$$y = w_0$$



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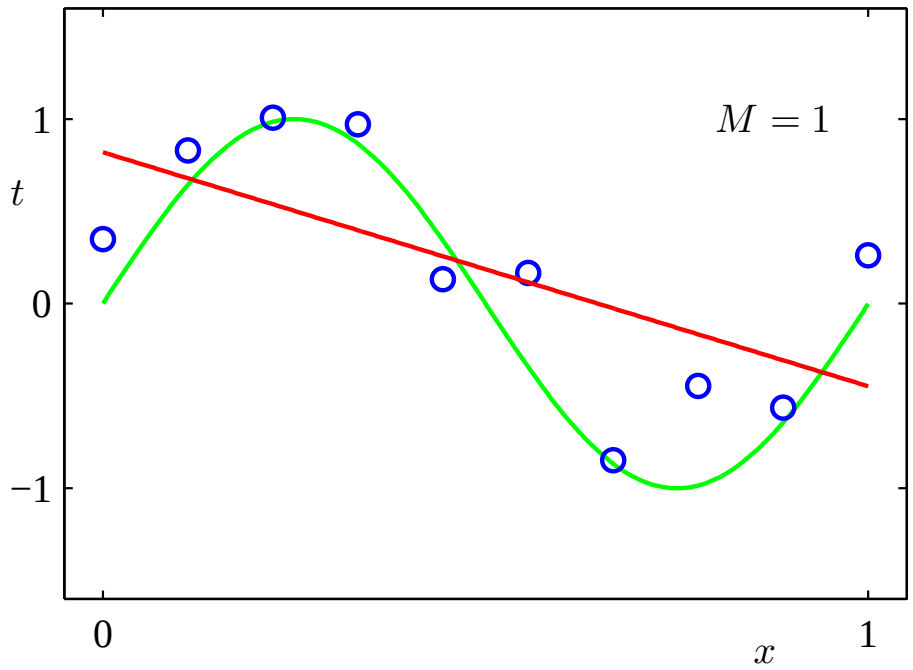
Fitting polynomials

$$y = w_0 + w_1 x$$



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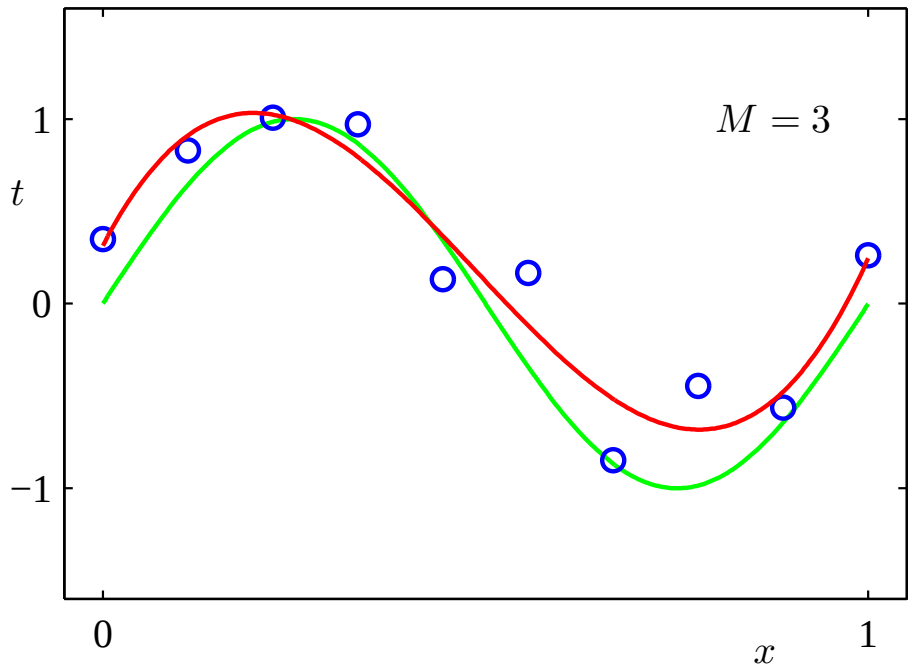
Fitting polynomials

$$y = w_0 + w_1 x + w_2 x^2 + w_3 x^3$$



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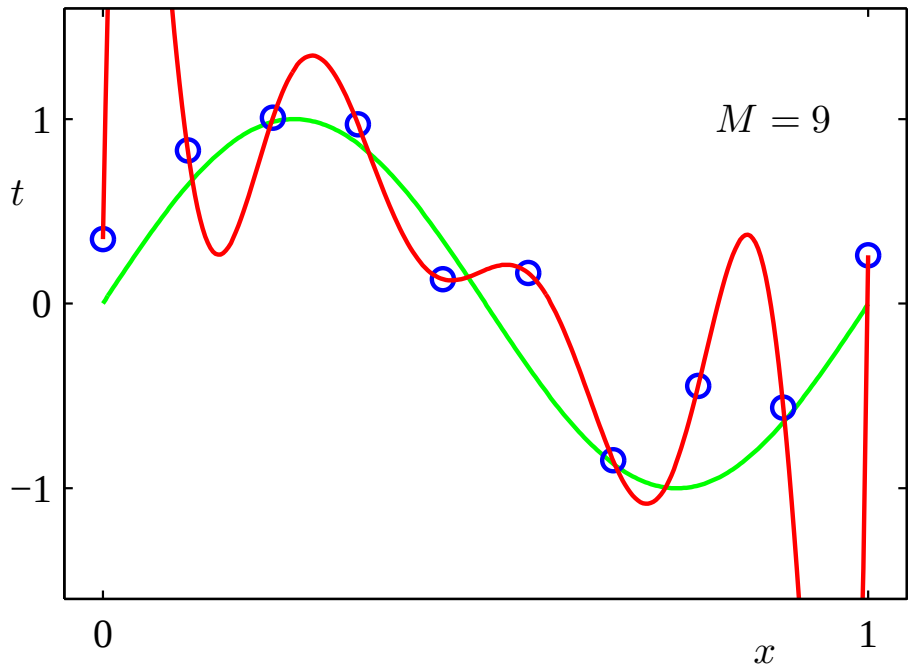
Fitting polynomials

$$y = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + \ldots + w_9 x^9$$



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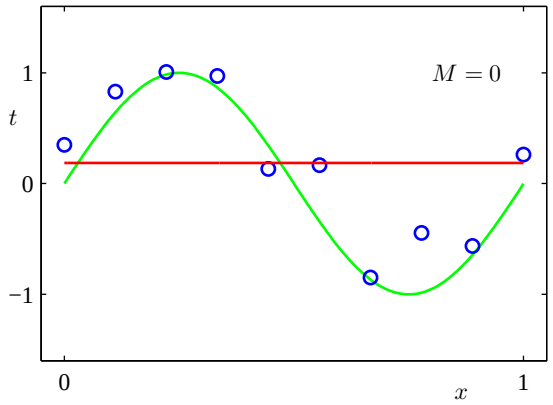
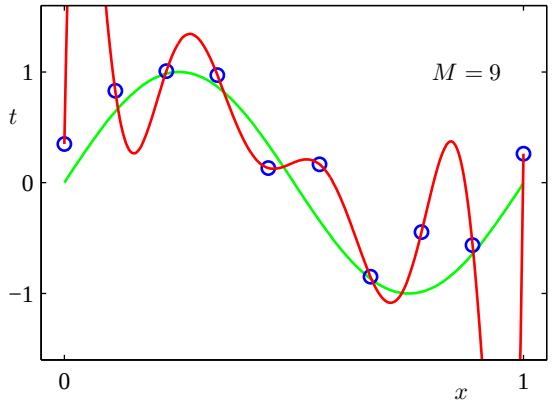
Generalization

Underfitting : The model is too simple - does not fit the data.

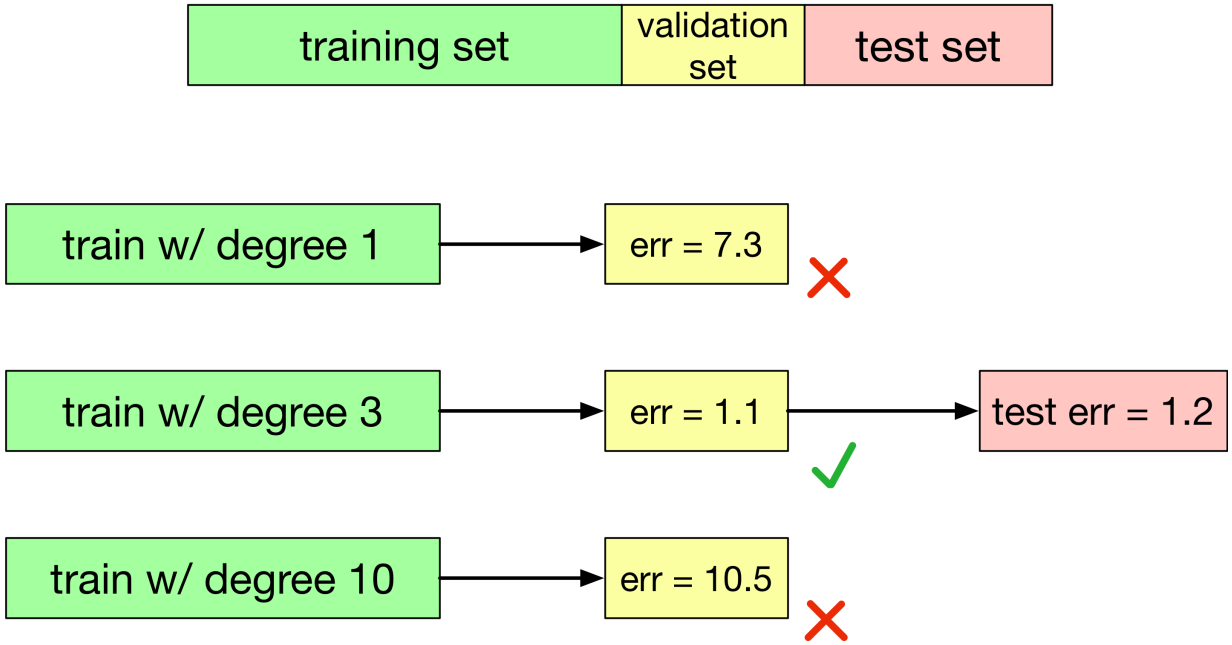


Overfitting : The model is too complex - fits perfectly, does not generalize.



Generalization

- We would like our models to generalize to data they haven't seen before
- The degree of the polynomial is an example of a hyperparameter, something we can't include in the training procedure itself
- We can tune hyperparameters using a validation set:



Foreshadowing

- Feature maps aren't a silver bullet:
  - It's not always easy to pick good features.
  - In high dimensions, polynomial expansions can get very large!
- Until the last few years, a large fraction of the effort of building a good machine learning system was feature engineering
- We'll see that neural networks are able to learn nonlinear functions directly, avoiding hand-engineering of features