STA 314: Statistical Methods for Machine Learning I

Lecture 4 - Ensembles & Linear Regression

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Today

- We will cover ensembling methods that combine multiple models and can perform better than the individual members.
  - We've seen individual models (KNN, decision trees)
- We will study bagging in particular, which trains models independently on random "resamples" of the training data.
- We will start our study of linear predictors, starting with linear regression.
- Highly recommend the course notes on the suggested reading: linear regression and calculus.

Bagging: Motivation

- What if we could somehow sample m independent training sets from p_{data}?
- In the previous discussion, we would have picked a separate predictor

$$\hat{y}_n^\star = \arg\min_{y \in \mathcal{H}} \hat{\mathcal{R}}[y, \mathcal{D}_n^{train}]$$

  averaged the losses $L(\hat{y}_n^\star(\mathbf{x}^{(i)}), t^{(i)})$ on the test set.
- What if instead we used the average prediction?

$$\bar{y}^\star(\mathbf{x}) = \frac{1}{m} \sum_{n=1}^{m} \hat{y}_n^\star(\mathbf{x})$$

Bagging: Motivation

- How does this affect the three terms of the expected loss?
  - **Bayes error: unchanged**, since we have no control over it
  - **Bias: unchanged**, since the averaged prediction has the same expectation

$$\mathbb{E}[\bar{y}^\star] = \mathbb{E}\left[\frac{1}{m}\sum_{n=1}^{m}\hat{y}_n^\star\right] = \mathbb{E}[\hat{y}_n^\star]$$

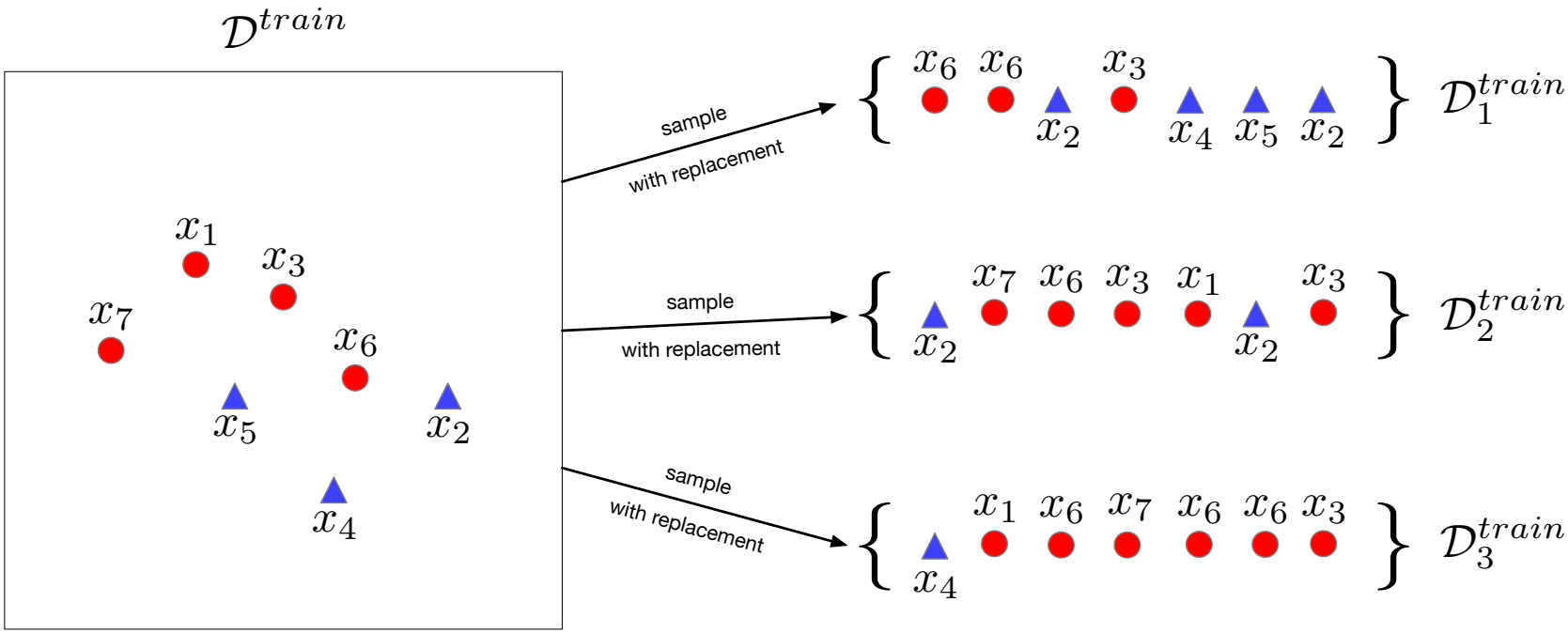
  - **Variance:** reduced, since we're averaging over independent samples

$$\mathrm{Var}[\bar{y}^\star] = \mathrm{Var}\left[\frac{1}{m}\sum_{n=1}^{m}\hat{y}_n^\star\right] = \frac{1}{m^2}\sum_{n=1}^{m}\mathrm{Var}[\hat{y}_n^\star] = \frac{1}{m}\mathrm{Var}[\hat{y}_n^\star].$$

Bagging: The Idea

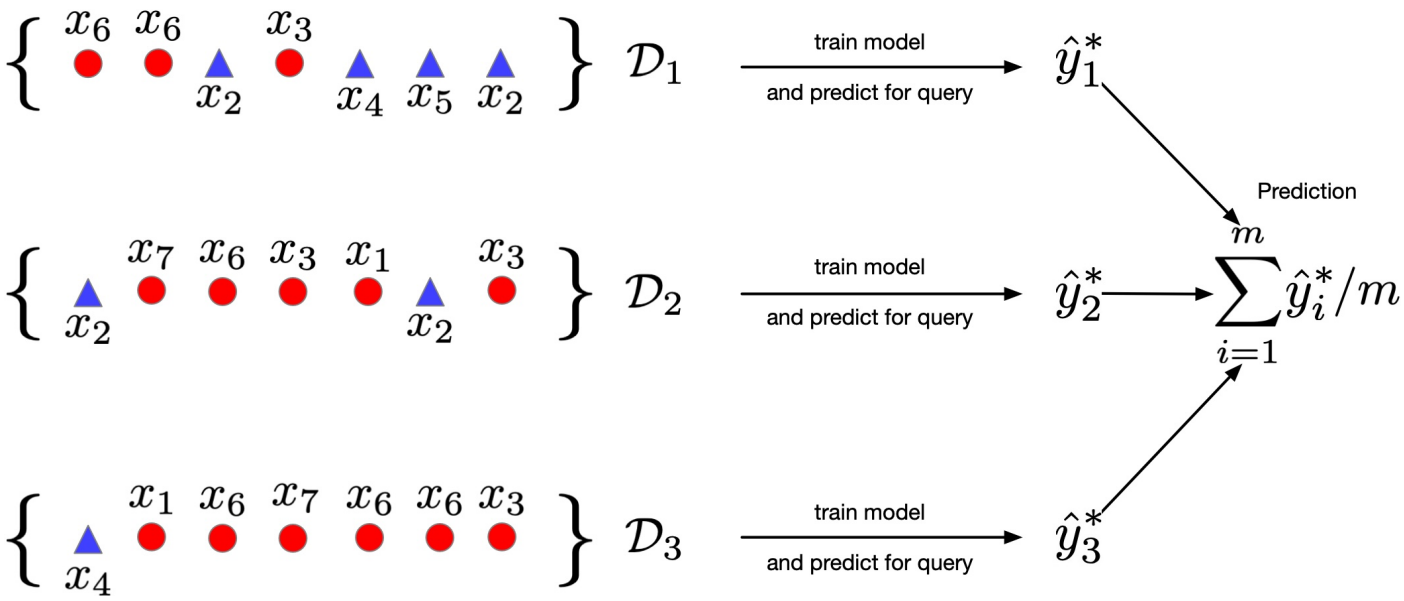
- In practice, the sampling distribution p_{data} is often finite or expensive to sample from.
- So training separate models on independently sampled datasets is very wasteful of data!
  - Why not train a single model on the union of all sampled datasets?
- Solution: given training set $\mathcal{D}^{train}$, use the empirical distribution $p_{\mathcal{D}^{train}}$ as a proxy for p_{data}. This is called bootstrap aggregation, or bagging .
  - Take a single dataset $\mathcal{D}^{train}$ with N examples.
  - Generate m new datasets ("resamples" or "bootstrap samples"), each by sampling N training examples from $\mathcal{D}^{train}$, with replacement.
  - Average the predictions of models trained on each of these datasets.
- The bootstrap is one of the most important ideas in all of statistics!

Bagging



in this example $N = 7$, $m = 3$

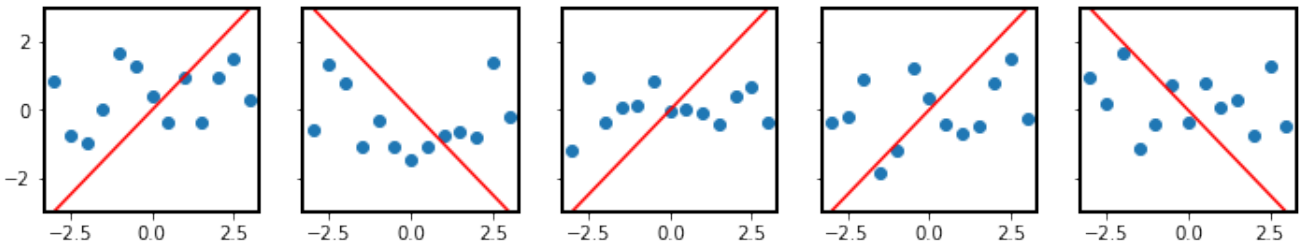
Bagging



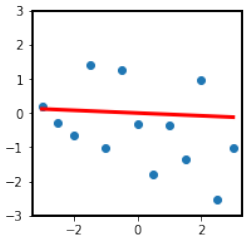
predicting on a query point x

Bagging: Effect on Hypothesis Space

- We saw that in case of squared error, bagging does not affect bias.
- But it can change the hypothesis space $\mathcal{H}$.
- Illustrative example:
  - $x \sim \mathcal{U}(-3, 3)$, $t \sim \mathcal{N}(0, 1)$
  - $\mathcal{H} = \{wx \mid w \in \{-1, 1\}\}$
  - Sampled datasets & fitted hypotheses:



  - Ensembled hypotheses (mean over 1000 samples):



    - The ensembled hypothesis is not in the original hypothesis space!

- This effect is often more pronounced when combining classifiers.

Bagging: Effect of Correlation

- Problem: the datasets are not independent, so we don't get the $1/m$ variance reduction.
  - If the sampled predictions $\hat{y}_n^*(\mathbf{x})$ have conditional variance $\sigma^2(\mathbf{x})$ and conditional correlation $\rho(\mathbf{x}) = \mathrm{Cov}(\hat{y}_i^*(\mathbf{x}), \hat{y}_j^*(\mathbf{x}) \mid \mathbf{x})/\sigma(\mathbf{x})^2$, then

$$\mathrm{Var}\left(\frac{1}{m}\sum_{n=1}^{m}\hat{y}_n^*(\mathbf{x})\middle|\mathbf{x}\right) = \frac{1}{m}(1-\rho(\mathbf{x}))\sigma(\mathbf{x})^2 + \rho(\mathbf{x})\sigma(\mathbf{x})^2.$$

- Ironically, it can be advantageous to introduce *additional* variability into your algorithm, as long as it reduces the correlation between samples.
  - Intuition: you want to invest in a diversified portfolio, not just one stock.
  - Can help to use average over multiple algorithms, or multiple configurations of the same algorithm.

Random Forests

- Random forests = bagged decision trees, with one extra trick to decorrelate the predictions
  - When choosing each node of the decision tree, choose a random set of d input features, and only consider splits on those features
- Random forests are probably the best black-box machine learning algorithm — they often work well with no tuning whatsoever.
  - one of the most widely used algorithms in Kaggle competitions

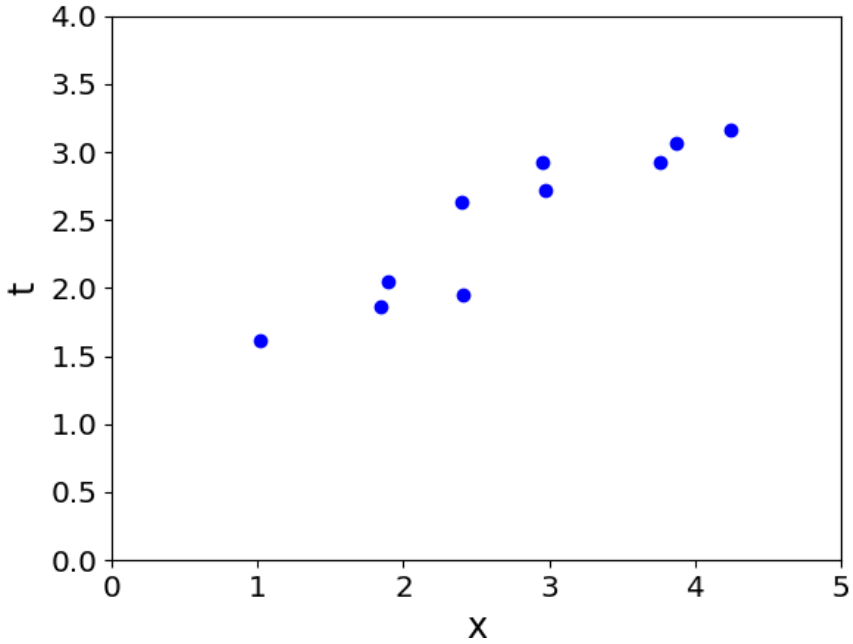
Bagging Summary

- Bagging reduces overfitting by averaging predictions.
- Used in most competition winners
  - Even if a single model is great, a small ensemble usually helps.
- Limitations:
  - Does not reduce bias in case of squared error.
  - There is still correlation between classifiers.
    - Random forest solution: Add more randomness.
  - Naive mixture (all members weighted equally).
    - If members are very different (e.g., different algorithms, different data sources, etc.), we can often obtain better results by using a principled approach to weighted ensembling.

Overview

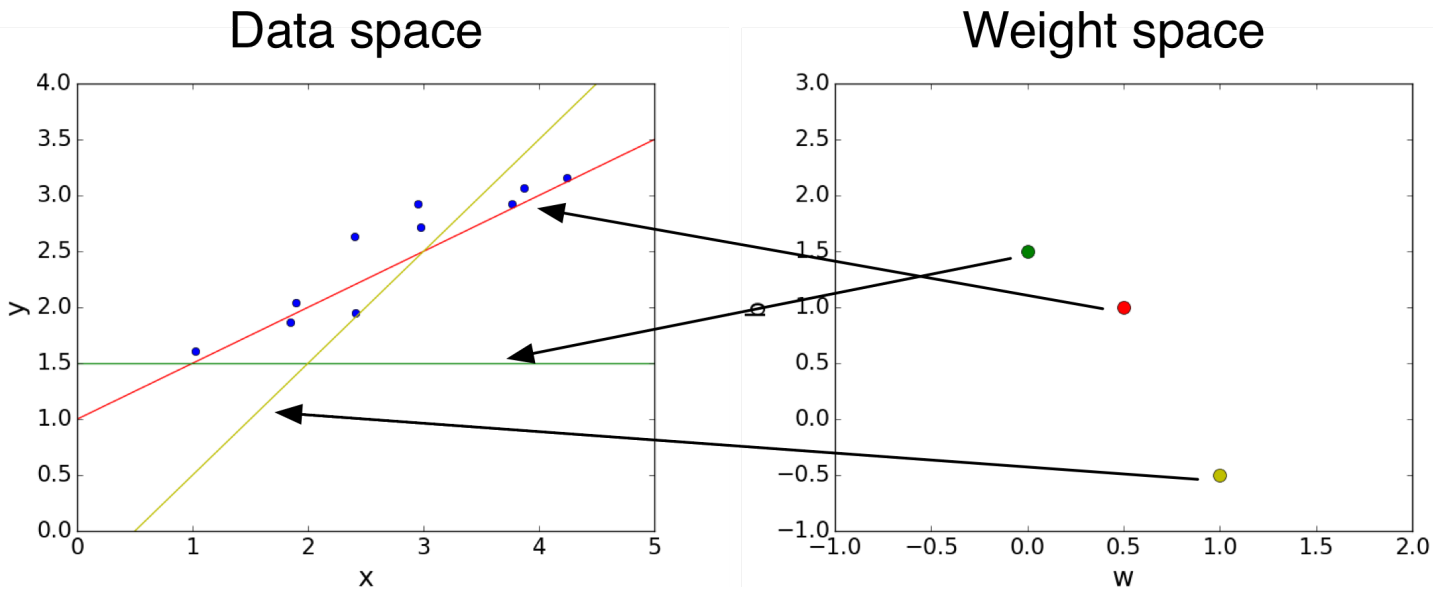
- So far, we've talked about *procedures* for learning.
  - KNN, decision trees, bagging
- For the remainder of this course, we'll take a more modular approach:
  - choose a model describing the relationships between variables of interest
  - define a loss function quantifying how bad is the fit to the data
  - choose a regularizer saying how much we prefer different candidate explanations
  - fit the model, e.g. using an optimization algorithm
- By mixing and matching these modular components, your ML skills become combinatorially more powerful!

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 inputs, and the $t^{(i)}$ are 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 the hypotheses

Problem Setup

- Loss function: squared error (says how bad the fit is)

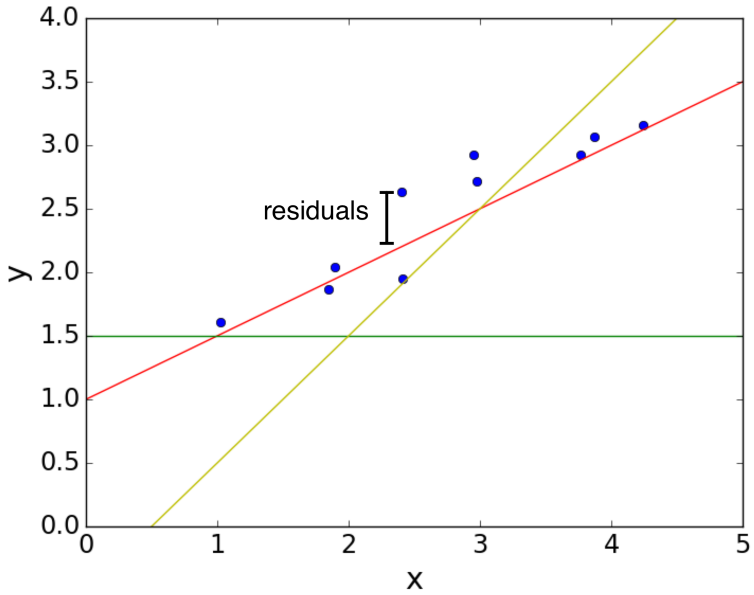
$$L(y, t) = \frac{1}{2}(y - t)^2$$

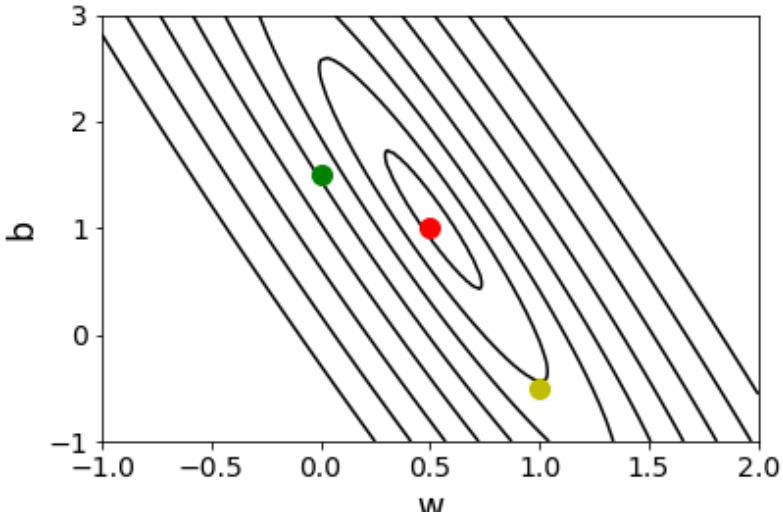
- $y - t$ is the residual, and we want to make this small in magnitude
- The $\frac{1}{2}$ factor is just to make the calculations convenient.
- Average loss function (some just called train or test loss or train or test error (if 0-1)):

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

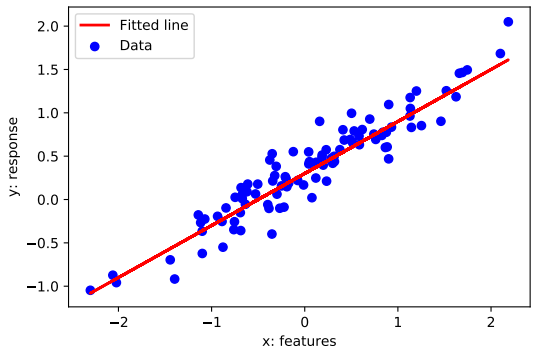
- You may sometimes see the term cost to mean train loss.

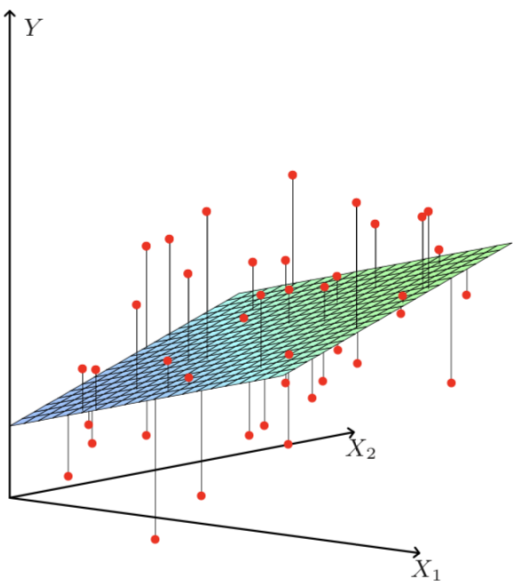
Problem Setup





What is linear? 1 feature vs D features





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

$$\hat{\mathcal{R}}(w, b) = \frac{1}{2N} \sum_{i=1}^{N} \left(wx^{(i)} + b - t^{(i)} \right)^2$$

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

$$\hat{\mathcal{R}}(\mathbf{w}, b) = \frac{1}{2N} \sum_{i=1}^{N} \left(\mathbf{w}^\top \mathbf{x}^{(i)} + b - t^{(i)} \right)^2$$

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

Vectorization

- Notation-wise, $\frac{1}{2N}\sum_{i=1}^{N}\left(y^{(i)}-t^{(i)}\right)^2$ gets messy if we expand $y^{(i)}$:

$$\frac{1}{2N}\sum_{i=1}^{N}\left(\left(\sum_{j=1}^{D} w_j x_j^{(i)} + b\right) - t^{(i)}\right)^2$$

- The code equivalent is to computing the prediction using a for loop:

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

- Excessive super/sub scripts are hard to work with, and Python loops are slow, so we vectorize algorithms by expressing them in terms of vectors and matrices.

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

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

- This is simpler and executes much faster:

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

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 (hardware support)
  - Matrix multiplication very fast on GPU (Graphics Processing Unit)

Switching in and out of vectorized form is a skill you gain with practice

- Some derivations are easier to do element-wise
- Some algorithms are easier to write/understand using for-loops and vectorize later for performance

Vectorization

- We can organize all the training examples into a design matrix $\mathbf{X}$ with one row per training example, and all the targets into the target 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:

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

Vectorization

- Computing the squared error across the whole dataset:

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

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

- Sometimes we may use $\hat{\mathcal{R}} = \frac{1}{2}\|\mathbf{y} - \mathbf{t}\|^2$, without a normalizer. This would correspond to the sum of losses, and not the averaged loss. The minimizer does not depend on N (but optimization might!).
- We can also add a column of 1's to design matrix, combine the bias and the weights, and conveniently write

$$\boldsymbol{X} = \begin{bmatrix} 1 & [\mathbf{x}^{(1)}]^\top \\ 1 & [\mathbf{x}^{(2)}]^\top \\ 1 & \vdots \end{bmatrix} \in \mathbb{R}^{N\times(D+1)} \qquad \boldsymbol{w} = \begin{bmatrix} b \\ w_1 \\ w_2 \\ \vdots \end{bmatrix} \in \mathbb{R}^{D+1}$$

Then, our predictions reduce to $\mathbf{y} = \mathbf{X}\mathbf{w}$.

Solving the Minimization Problem

We defined a train loss. This is what we'd like to minimize.

Two commonly applied mathematical approaches:

- Algebraic, e.g., using inequalities:
  - to show z^* minimizes $f(z)$, show that $\forall z, f(z) \geq f(z^*)$
  - to show that $a = b$, show that $a \geq b$ and $b \geq a$
- Calculus: 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 (or equivalently the gradient).

Solutions may be direct or iterative

- Sometimes we can directly find provably optimal parameters (e.g. set the gradient to zero and solve in closed form). We call this a direct solution.
- We may also use optimization techniques that iteratively get us closer to the solution. We will get back to this soon.

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:

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

- Train loss derivatives (average over data points):

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

Direct solution

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

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

- If $\partial \hat{\mathcal{R}} / \partial w_j \neq 0$, you could reduce the train loss by changing w_j.
- This turns out to give a system of linear equations, which we can solve efficiently.
- Let's see what this looks like, assuming for simplicity that we set $b = 0$ (we can always add a dummy dimension to our data)

Direct solution

- We seek $\mathbf{w}$ to minimize $\hat{\mathcal{R}}(\mathbf{w}) = \frac{1}{2}||\mathbf{X}\mathbf{w} - \mathbf{t}||^2$
- Consider the vector of partial derivatives, or gradient:

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

- Setting this to 0 (**see course notes for additional details**) we get:

$$\frac{\partial \hat{\mathcal{R}}}{\partial \mathbf{w}} = \mathbf{X}^\top \mathbf{X}\mathbf{w} - \mathbf{X}^\top \mathbf{t} = \mathbf{0}$$

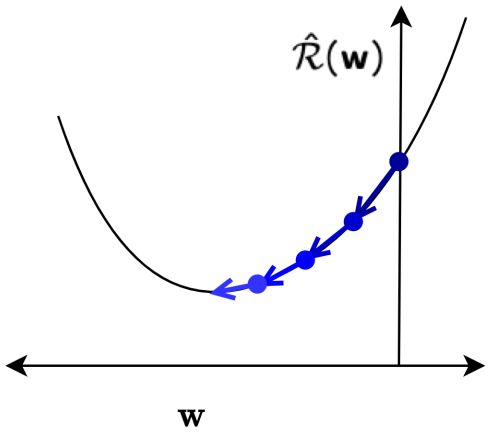
- From which we get the following train loss optimal weights (minimize average loss on train):

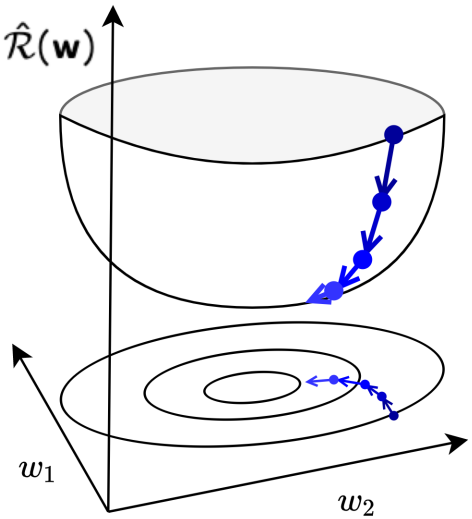
$$\hat{\mathbf{w}}^* = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{t}$$

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

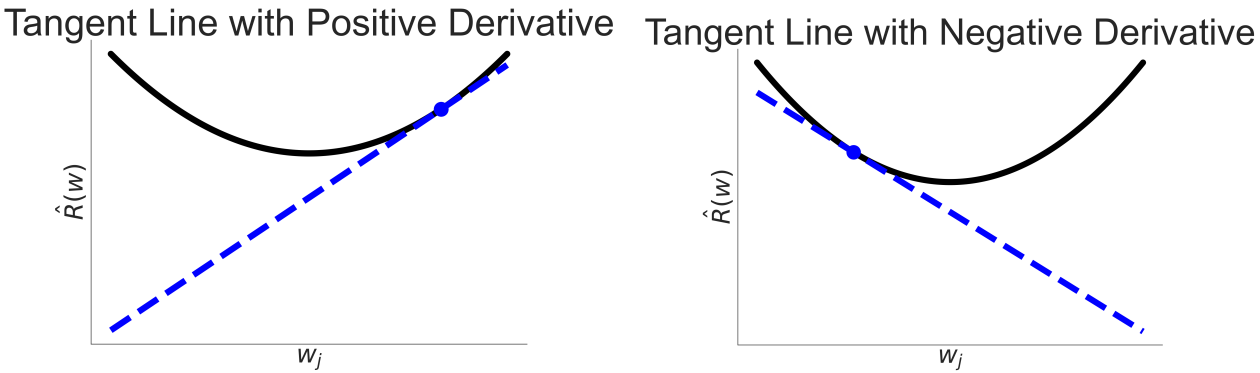
Gradient Descent

- Now let's see a second way to minimize the train loss which is more broadly applicable: gradient descent.
- Many times, we do not have a direct solution: Taking derivatives of $\hat{\mathcal{R}}$ w.r.t $\mathbf{w}$ and setting them to 0 doesn't have an explicit solution.
- 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.





Gradient Descent



First derivatives give us rates of change

- if $\partial\hat{\mathcal{R}}/\partial w_j > 0$, then decreasing w_j decreases $\hat{\mathcal{R}}$.
- if $\partial\hat{\mathcal{R}}/\partial w_j < 0$, then increasing w_j decreases $\hat{\mathcal{R}}$.

Gradient Descent

- The following update always decreases the train loss for small enough α (unless $\partial\hat{\mathcal{R}}/\partial w_j = 0$):

$$w_j \leftarrow w_j - \alpha \frac{\partial \hat{\mathcal{R}}}{\partial w_j}$$

- $\alpha > 0$ is a learning rate (or step size). 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.
  - If train loss is the sum of N individual losses rather than their average, smaller learning rate will be needed ($\alpha' = \alpha/N$).

Gradient descent

- Update rule in vector form:

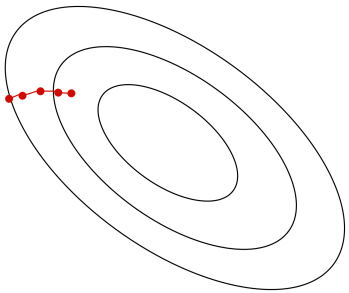
$$\begin{aligned}\mathbf{w} &\leftarrow \mathbf{w} - \alpha \frac{\partial \hat{\mathcal{R}}}{\partial \mathbf{w}} \\ &= \mathbf{w} - \frac{\alpha}{N} \sum_{i=1}^{N} (y^{(i)} - t^{(i)}) \, \mathbf{x}^{(i)}\end{aligned}$$

Gradient Descent for Linear Regression

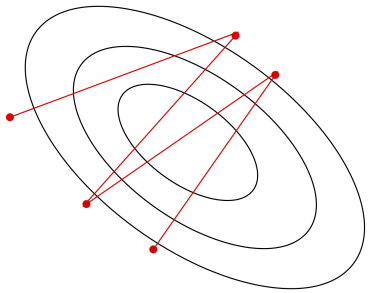
- The squared error loss of linear regression is a convex function.
- Even for linear regression, where there is a direct solution, we sometimes need to use GD.
- Why gradient descent, if we can find the optimum directly?
  - GD can be applied to a much broader set of models
  - GD can be easier to implement than direct solutions
  - For regression in high-dimensional space, GD is more efficient than direct solution
    - Linear regression solution: $(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{t}$
    - Matrix inversion is an $\mathcal{O}(D^3)$ algorithm
    - Each GD update costs $\mathcal{O}(ND)$
    - Or less with stochastic GD (SGD, in a few slides)
    - Huge difference if $D \gg 1$

Learning Rate (Step Size)

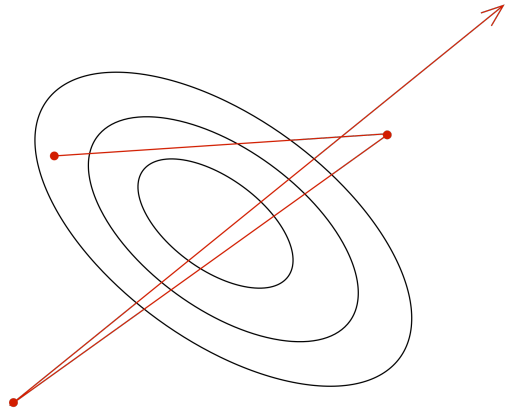
- In gradient descent, the learning rate α is a hyperparameter we need to tune. Here are some things that can go wrong:



α too small:
slow progress



α too large:
oscillations

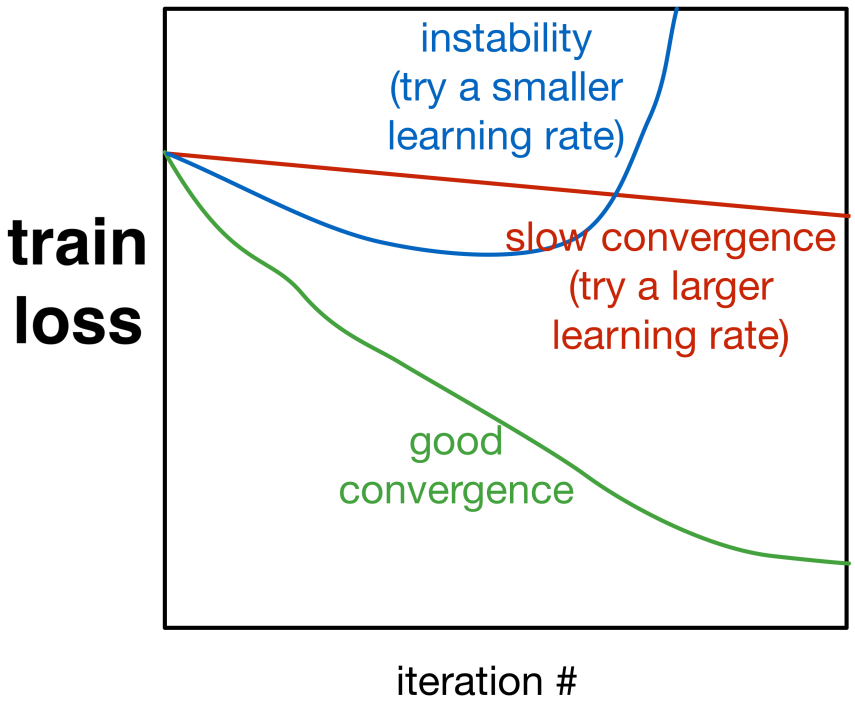


α much too large:
instability

- Good values are typically between 0.001 and 0.1. You should do a grid search if you want good performance (i.e. try $0.1, 0.03, 0.01, \ldots$).

Training Curves

- To diagnose optimization problems, it's useful to look at training curves: plot the train loss as a function of iteration.



- Warning: in general, it's very hard to tell from the training curves whether an optimizer has converged. They can reveal major problems, but they can't guarantee convergence.

Gradient descent

Visualization (we aren't covering in class):

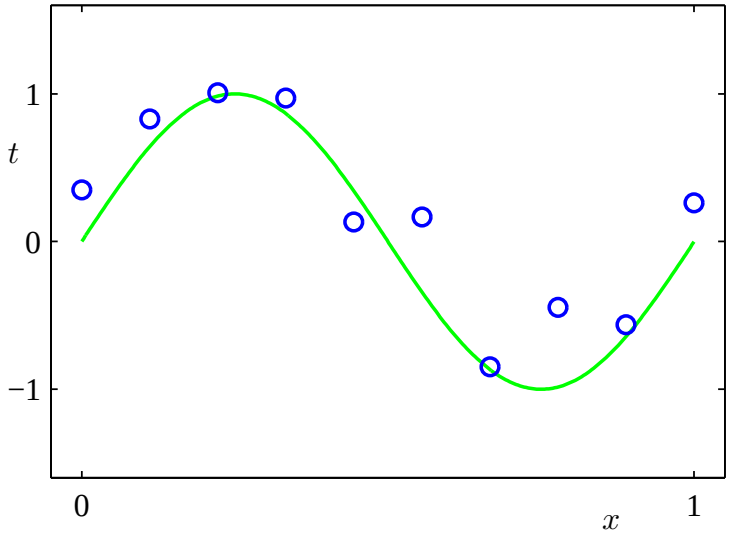
`http://www.cs.toronto.edu/~guerzhoy/321/lec/W01/linear_regression.pdf#page=21`

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

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

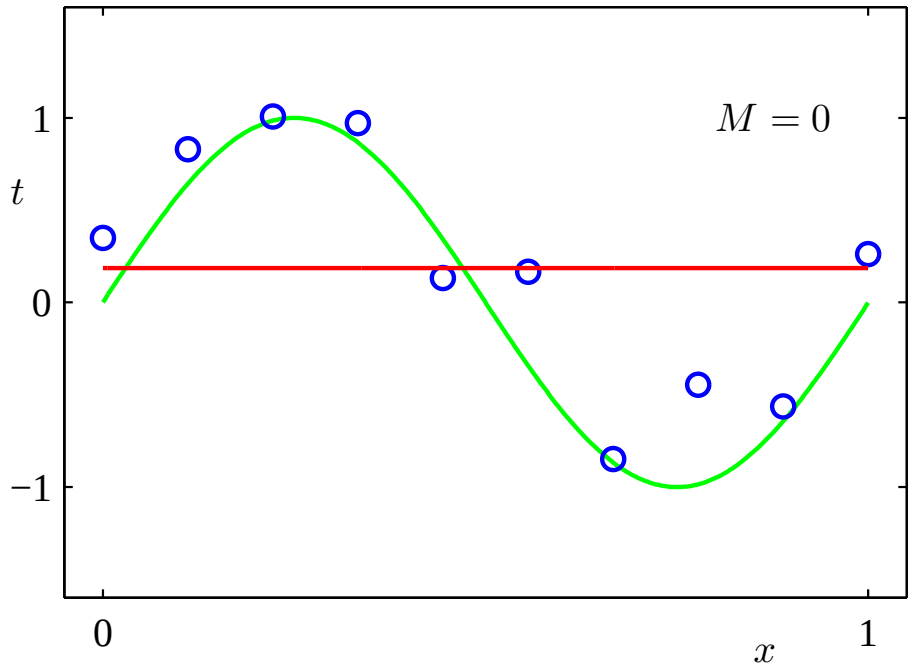
- Polynomial regression model:

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

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

Fitting polynomials

$y = w_0$



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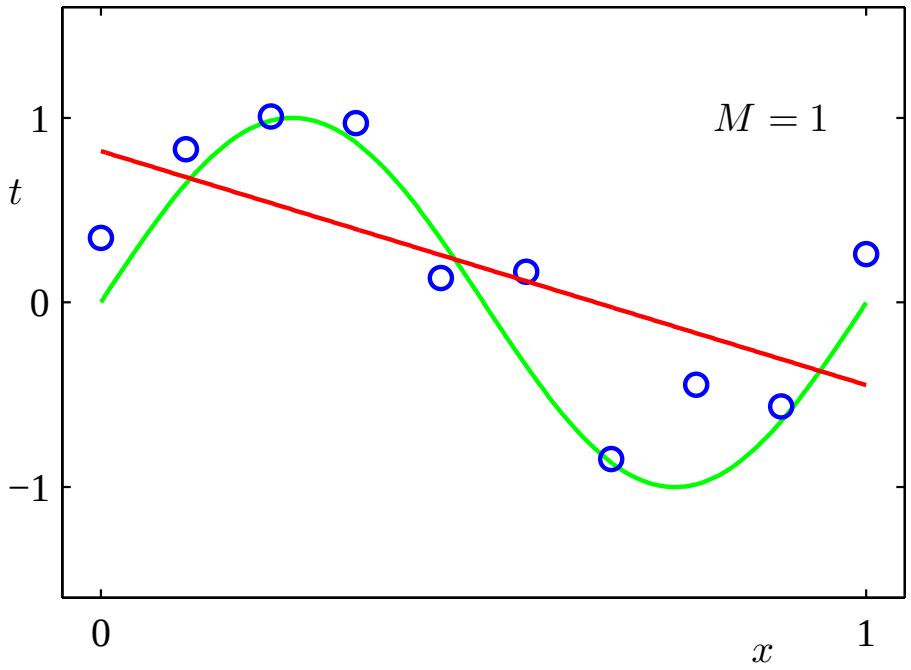
Fitting polynomials

$$y = w_0 + w_1 x$$



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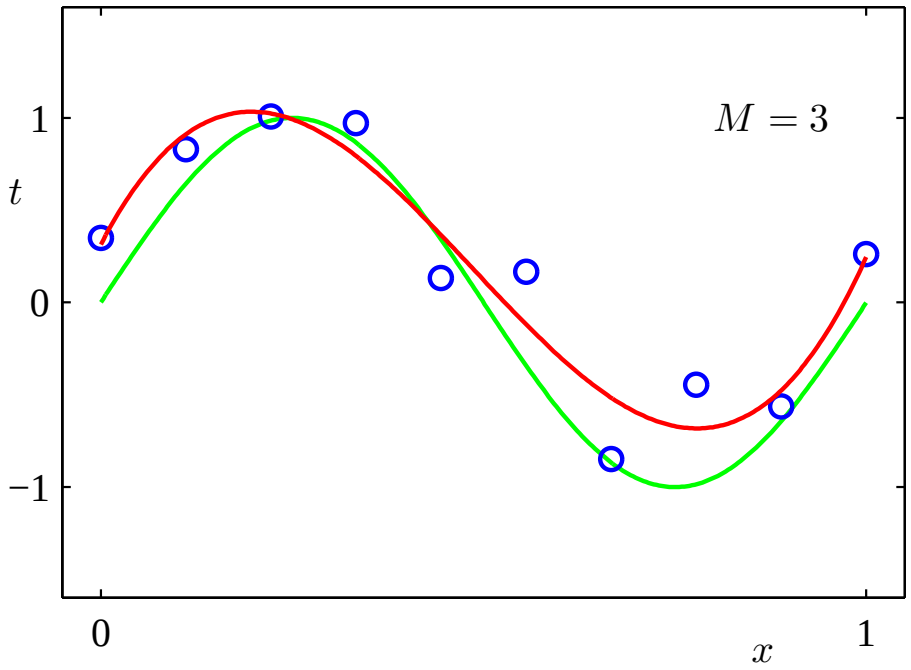
Fitting polynomials

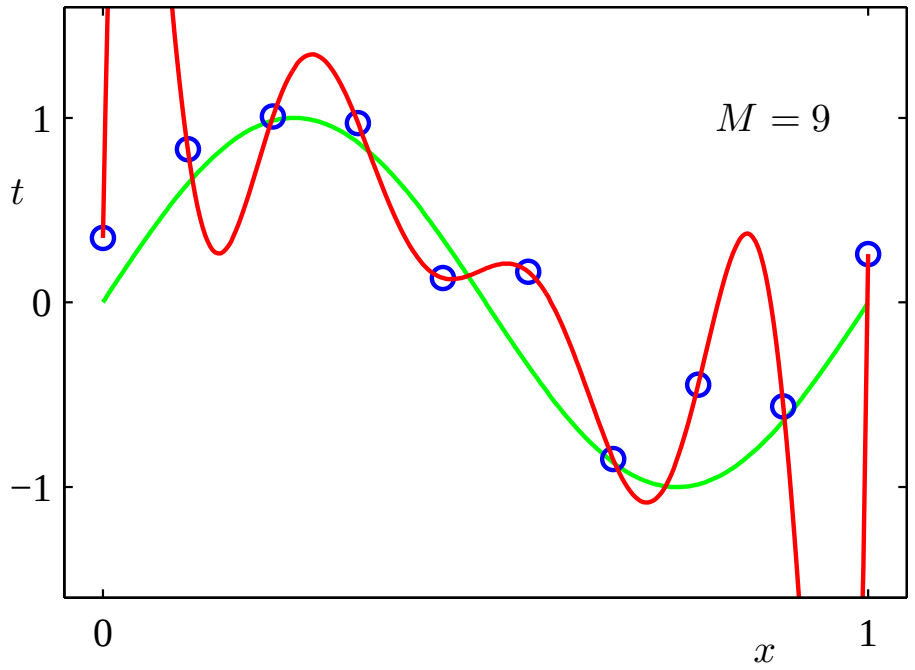
$$y = w_0 + w_1 x + w_2 x^2 + w_3 x^3$$



-Pattern Recognition and Machine Learning, Christopher Bishop.

Fitting polynomials

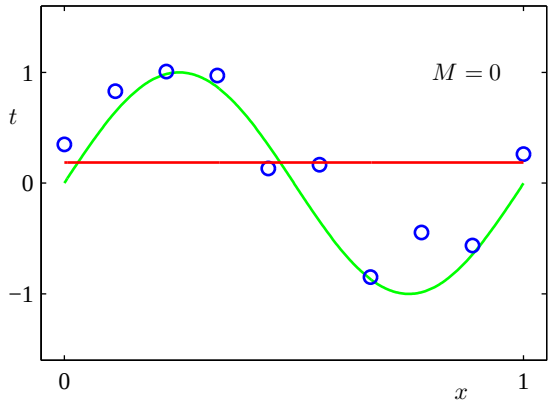
$$y = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + \ldots + w_9 x^9$$



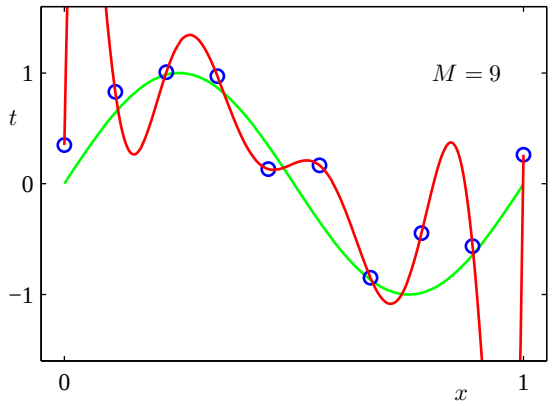
-Pattern Recognition and Machine Learning, Christopher Bishop.

Generalization

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

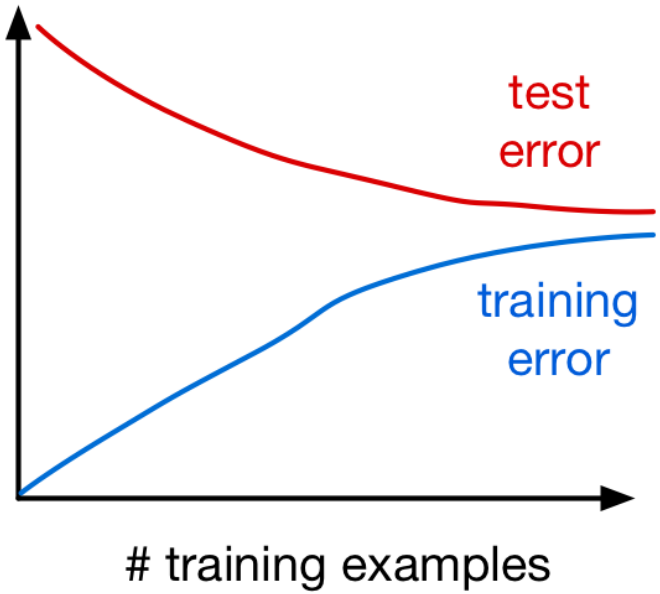


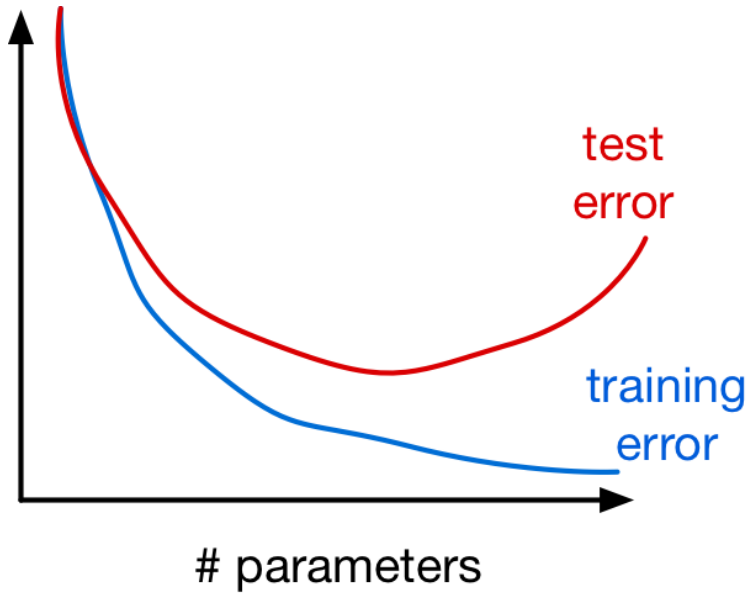
Overfitting : model is too complex — fits perfectly, does not generalize.



Generalization

- Training and test error as a function of # training examples and # parameters:



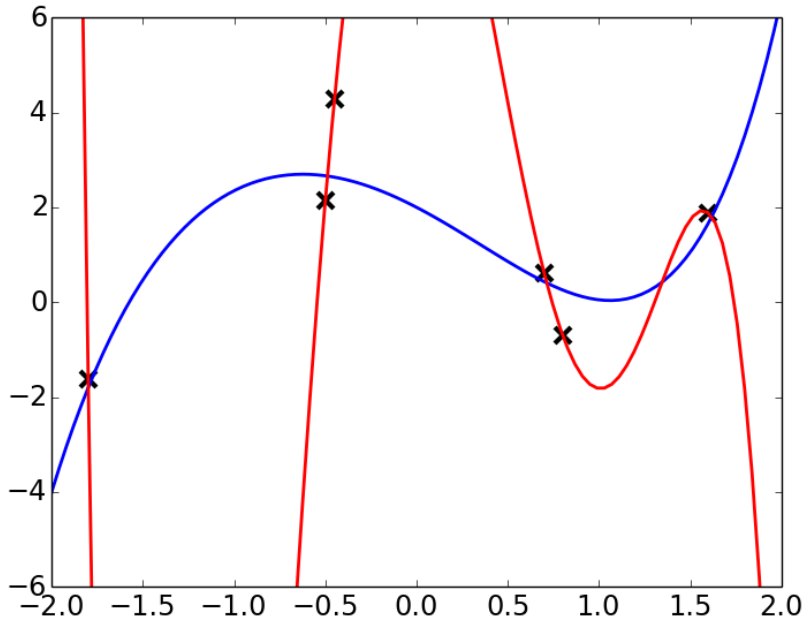


Regularization

- The degree of the polynomial is a hyperparameter, just like k in KNN. We can tune it using a validation set.
- But restricting the size of the model is a crude solution, since you'll never be able to learn a more complex model, even if the data support it.
- Another approach: keep the model large, but regularize it
  - Regularizer: a function that quantifies how much we prefer one hypothesis vs. another

L^2 Regularization

Observation: polynomials that overfit often have large coefficients.



$$y = 0.1x^5 + 0.2x^4 + 0.75x^3 - x^2 - 2x + 2$$

$$y = -7.2x^5 + 10.4x^4 + 24.5x^3 - 37.9x^2 - 3.6x + 12$$

So let's try to keep the coefficients small.

L^2 Regularization

Another reason we want weights to be small:

- Suppose inputs x_1 and x_2 are nearly identical for all training examples. The following two hypotheses make nearly the same predictions:

$$\mathbf{w} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad \mathbf{w} = \begin{pmatrix} -9 \\ 11 \end{pmatrix}$$

- But the second network might make weird predictions if the test distribution is slightly different (e.g. x_1 and x_2 match less closely).

L^2 (or ℓ_2) Regularization

- We can encourage the weights to be small by choosing as our regularizer the L^2 penalty.

$$\phi(\mathbf{w}) = \frac{1}{2}\|\mathbf{w}\|_2^2 = \frac{1}{2}\sum_j w_j^2.$$

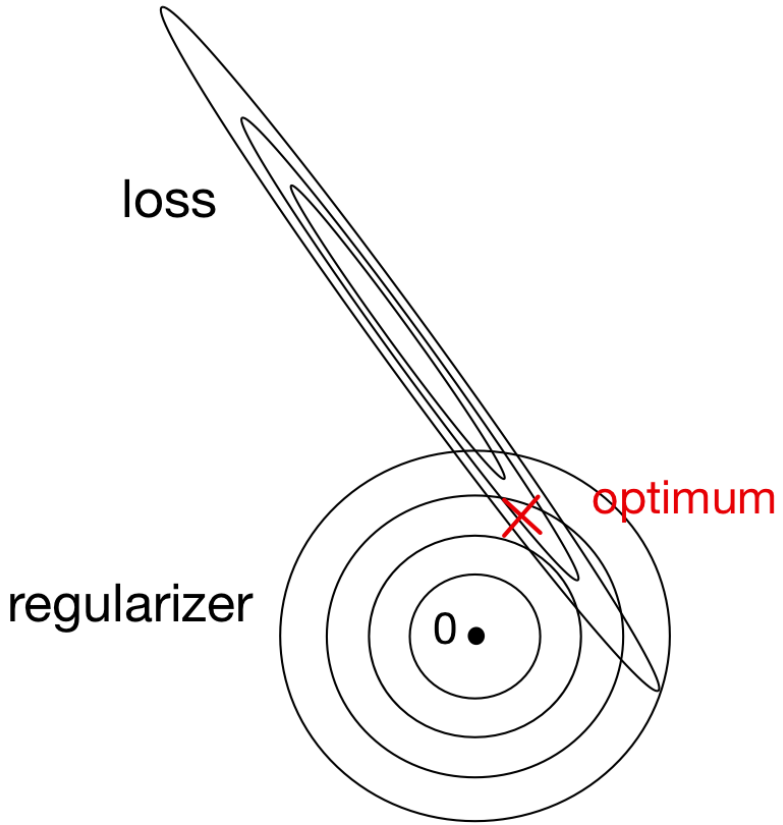
  - Note: To be precise, the L^2 norm is Euclidean distance, so we're regularizing the *squared* L^2 norm.
- The regularized train loss makes a tradeoff between fit to the data and the norm of the weights.

$$\hat{\mathcal{R}}_{\text{reg}}(\mathbf{w}) = \hat{\mathcal{R}}(\mathbf{w}) + \lambda\phi(\mathbf{w}) = \hat{\mathcal{R}}(\mathbf{w}) + \frac{\lambda}{2}\sum_j w_j^2$$

- If you fit training data poorly, $\hat{\mathcal{R}}$ is large. If your optimal weights have high values, ϕ is large.
- Large λ penalizes weight values more.
- Like M, λ is a hyperparameter we can tune with a validation set.

L^2 (or ℓ_2) Regularization

- The geometric picture:



L^2 Regularized Least Squares: Ridge regression

For the least squares problem, we have $\hat{\mathcal{R}}(\mathbf{w}) = \frac{1}{2N}\|\mathbf{X}\mathbf{w} - \mathbf{t}\|^2$.

- When $\lambda > 0$ (with regularization), regularized train loss gives

$$\mathbf{w}_\lambda^{\text{Ridge}} = \operatorname*{argmin}_{\mathbf{w}} \hat{\mathcal{R}}_{\text{reg}}(\mathbf{w}) = \operatorname*{argmin}_{\mathbf{w}} \frac{1}{2N}\|\mathbf{X}\mathbf{w} - \mathbf{t}\|_2^2 + \frac{\lambda}{2}\|\mathbf{w}\|_2^2$$
$$= (\mathbf{X}^\top\mathbf{X} + \lambda N\mathbf{I})^{-1}\mathbf{X}^\top\mathbf{t}$$

- The case $\lambda = 0$ (no regularization) reduces to least squares solution!
- Note that it is also common to formulate this problem as $\operatorname{argmin}_{\mathbf{w}} \frac{1}{2}\|\mathbf{X}\mathbf{w} - \mathbf{t}\|_2^2 + \frac{\lambda}{2}\|\mathbf{w}\|_2^2$ in which case the solution is $\mathbf{w}_\lambda^{\text{Ridge}} = (\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^\top\mathbf{t}$.

Gradient Descent under the L^2 Regularization

- Gradient descent update to minimize $\hat{\mathcal{R}}$:

$$\mathbf{w} \leftarrow \mathbf{w} - \alpha \frac{\partial}{\partial \mathbf{w}} \hat{\mathcal{R}}$$

- The gradient descent update to minimize the L^2 regularized train loss $\hat{\mathcal{R}} + \lambda \mathcal{R}$ results in weight decay:

$$\begin{aligned}
\mathbf{w} &\leftarrow \mathbf{w} - \alpha \frac{\partial}{\partial \mathbf{w}} \left(\hat{\mathcal{R}} + \lambda \phi \right) \\
&= \mathbf{w} - \alpha \left(\frac{\partial \hat{\mathcal{R}}}{\partial \mathbf{w}} + \lambda \frac{\partial \phi}{\partial \mathbf{w}} \right) \\
&= \mathbf{w} - \alpha \left(\frac{\partial \hat{\mathcal{R}}}{\partial \mathbf{w}} + \lambda \mathbf{w} \right) \\
&= (1 - \alpha\lambda)\mathbf{w} - \alpha \frac{\partial \hat{\mathcal{R}}}{\partial \mathbf{w}}
\end{aligned}$$

Conclusion so far

Linear regression exemplifies recurring themes of this course:

- choose a model and a loss function
- formulate an optimization problem
- solve the minimization problem using one of two strategies
  - direct solution (set derivatives to zero)
  - gradient descent (next topic)
- vectorize the algorithm, i.e. represent in terms of linear algebra
- make a linear model more powerful using features
- improve the generalization by adding a regularizer