CSCI567 Machine Learning (Fall 2023)

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Outline

Regression

Predicting a continuous outcome variable using past observations

- Predicting future temperature (last lecture)
- Predicting the amount of rainfall
- Predicting the demand of a product
- Predicting the sale price of a house
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- continuous vs discrete
- measure *prediction errors* differently.
- lead to quite different learning algorithms.

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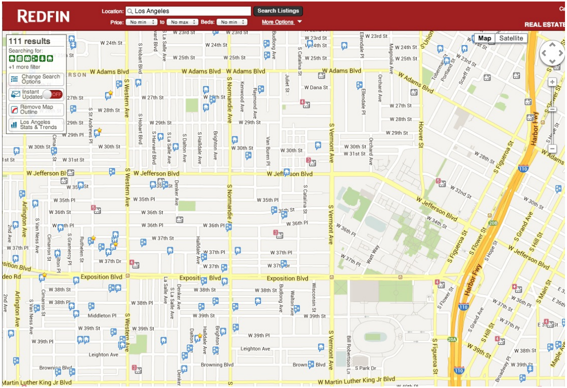
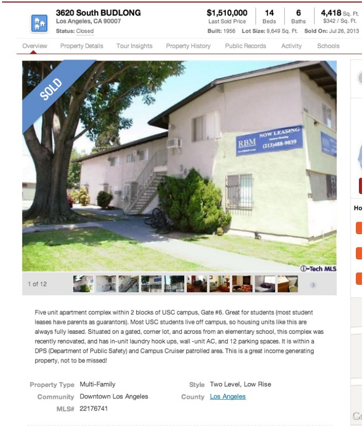
Linear Regression: regression with linear models

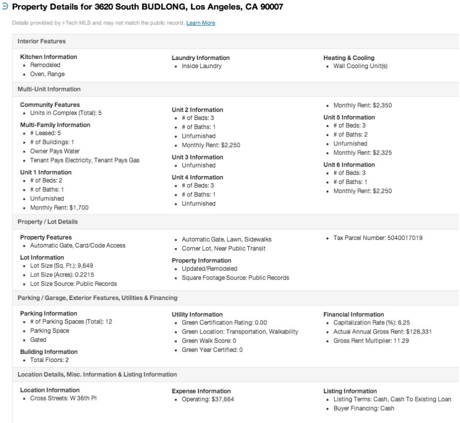
Ex: Predicting the sale price of a house

Retrieve historical sales records (training data)

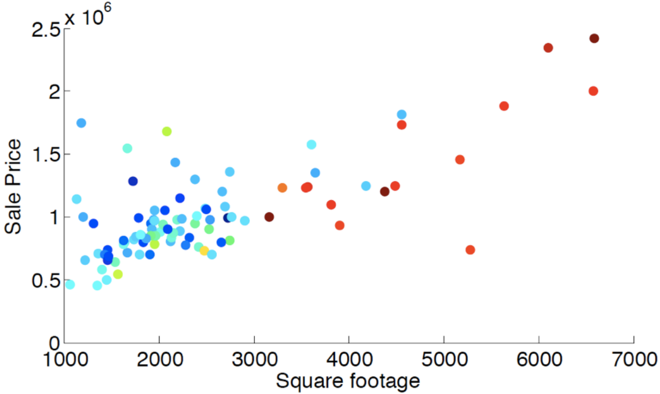


Features used to predict



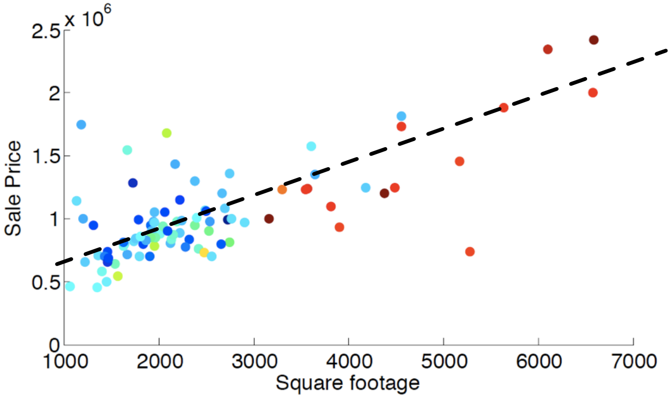


Correlation between square footage and sale price



Possibly linear relationship

Sale price ≈ **price_per_sqft** × square_footage + **fixed_expense**



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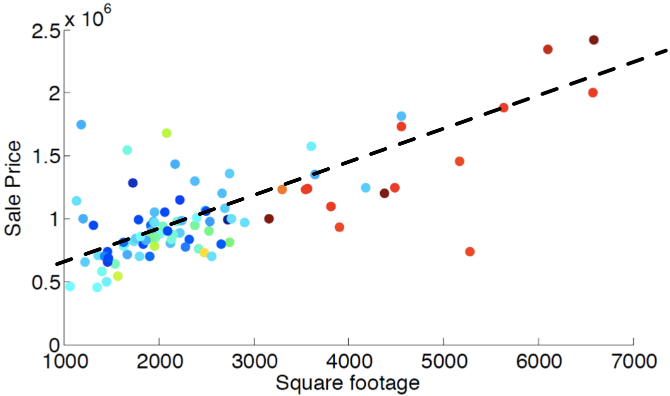
(*slope*) (*intercept*)



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- training set ✓

Example

Predicted price = **price_per_sqft** × square_footage + **fixed_expense**

one model: price_per_sqft = 0.3K, fixed_expense = 210K

sqft	sale price (K)	prediction (K)	squared error
2000	810	810	0
2100	907	840	67^2
1100	312	540	228^2
5500	2,600	1,860	740^2
$\cdots$	$\cdots$	$\cdots$	$\cdots$
Total			$0 + 67^2 + 228^2 + 740^2 + \cdots$

Adjust price_per_sqft and fixed_expense such that the total squared error is minimized.

Formal setup for linear regression

Input: $\boldsymbol{x} \in \mathbb{R}^{\mathsf{D}}$ (features, covariates, context, predictors, etc)

Output: $y \in \mathbb{R}$ (responses, targets, outcomes, etc)

Training data: $\mathcal{D} = \{(\boldsymbol{x}_n, y_n), n = 1, 2, \ldots, \mathsf{N}\}$

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- sometimes just use $\boldsymbol{w}, \boldsymbol{x}, \mathsf{D}$ for $\tilde{\boldsymbol{w}}, \tilde{\boldsymbol{x}}, \mathsf{D} + 1$!

Goal

Minimize total squared error

$$\sum_n (f(\boldsymbol{x}_n) - y_n)^2 = \sum_n (\tilde{\boldsymbol{x}}_n^{\mathrm{T}} \tilde{\boldsymbol{w}} - y_n)^2$$

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Minimize total squared error

- **Residual Sum of Squares** (RSS), a function of $\tilde{\boldsymbol{w}}$

$$\mathrm{RSS}(\tilde{\boldsymbol{w}}) = \sum_n \left(f(\boldsymbol{x}_n) - y_n\right)^2 = \sum_n (\tilde{\boldsymbol{x}}_n^{\mathrm{T}} \tilde{\boldsymbol{w}} - y_n)^2$$

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- find $\tilde{\boldsymbol{w}}^* = \operatorname*{argmin}_{\tilde{\boldsymbol{w}} \in \mathbb{R}^{\mathsf{D}+1}} \mathrm{RSS}(\tilde{\boldsymbol{w}})$, i.e. **least squares solution** (more generally called **empirical risk minimizer**)

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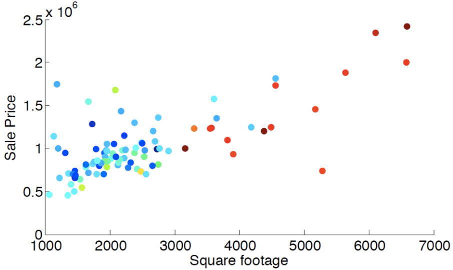
- *reduce machine learning to optimization*

- in principle can apply any optimization algorithm, but linear regression admits a *closed-form solution*

Warm-up: D $= 0$

Only one parameter w_0: constant prediction $f(x) = w_0$



f is a horizontal line, where should it be?

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Optimization objective becomes

$$\mathrm{RSS}(w_0) = \sum_n (w_0 - y_n)^2 \qquad \text{(it's a } \textit{quadratic } aw_0^2 + bw_0 + c\text{)}$$

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Exercise: what if we use absolute error instead of squared error?

Warm-up: $\mathrm{D} = 1$

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General approach: find *stationary points*, i.e., points with *zero gradient*

$$\begin{cases} \frac{\partial \mathrm{RSS}(\tilde{\boldsymbol{w}})}{\partial w_0} = 0 \\ \frac{\partial \mathrm{RSS}(\tilde{\boldsymbol{w}})}{\partial w_1} = 0 \end{cases} \Rightarrow \begin{array}{ll} \sum_n (w_0 + w_1 x_n - y_n) & = 0 \\ \sum_n (w_0 + w_1 x_n - y_n) x_n & = 0 \end{array}$$

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Least square solution for D $= 1$

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(assuming the matrix is invertible)

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- not true in general

General least square solution

Objective

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Again, find stationary points (**multivariate calculus**)

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$$\nabla \mathrm{RSS}(\tilde{\boldsymbol{w}}) = 2 \sum_n \tilde{\boldsymbol{x}}_n (\tilde{\boldsymbol{x}}_n^{\mathrm{T}} \tilde{\boldsymbol{w}} - y_n) \propto \left(\sum_n \tilde{\boldsymbol{x}}_n \tilde{\boldsymbol{x}}_n^{\mathrm{T}} \right) \tilde{\boldsymbol{w}} - \sum_n \tilde{\boldsymbol{x}}_n y_n$$

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where

$$\tilde{\boldsymbol{X}} = \begin{pmatrix} \tilde{\boldsymbol{x}}_1^{\mathrm{T}} \\ \tilde{\boldsymbol{x}}_2^{\mathrm{T}} \\ \vdots \\ \tilde{\boldsymbol{x}}_{\mathsf{N}}^{\mathrm{T}} \end{pmatrix} \in \mathbb{R}^{\mathsf{N} \times (D+1)}, \quad \boldsymbol{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_{\mathsf{N}} \end{pmatrix} \in \mathbb{R}^{\mathsf{N}}$$

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where

$$\tilde{\boldsymbol{X}} = \begin{pmatrix} \tilde{\boldsymbol{x}}_1^{\mathrm{T}} \\ \tilde{\boldsymbol{x}}_2^{\mathrm{T}} \\ \vdots \\ \tilde{\boldsymbol{x}}_{\mathsf{N}}^{\mathrm{T}} \end{pmatrix} \in \mathbb{R}^{\mathsf{N} \times (D+1)}, \quad \boldsymbol{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_{\mathsf{N}} \end{pmatrix} \in \mathbb{R}^{\mathsf{N}}$$

General least square solution

$$(\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}})\tilde{\boldsymbol{w}} - \tilde{\boldsymbol{X}}^{\mathrm{T}}\boldsymbol{y} = \boldsymbol{0} \quad \Rightarrow \quad \tilde{\boldsymbol{w}}^* = (\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}})^{-1}\tilde{\boldsymbol{X}}^{\mathrm{T}}\boldsymbol{y}$$

assuming $\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}}$ (**covariance matrix**) is invertible for now.

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$$\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}} = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ x_1 & x_2 & \cdots & x_{\mathsf{N}} \end{pmatrix} \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \cdots & \cdots \\ 1 & x_{\mathsf{N}} \end{pmatrix} = \begin{pmatrix} N & \sum_n x_n \\ \sum_n x_n & \sum_n x_n^2 \end{pmatrix}$$

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when $\mathsf{D} = 0$**:** $(\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}})^{-1} = \frac{1}{N}$, $\tilde{\boldsymbol{X}}^{\mathrm{T}}\boldsymbol{y} = \sum_n y_n$

Another approach

RSS is a **quadratic**, so let's complete the square:

$$\mathrm{RSS}(\tilde{\boldsymbol{w}}) = \sum_n (\tilde{\boldsymbol{w}}^{\mathrm{T}} \tilde{\boldsymbol{x}}_n - y_n)^2 = \|\tilde{\boldsymbol{X}} \tilde{\boldsymbol{w}} - \boldsymbol{y}\|_2^2$$

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So $\tilde{\boldsymbol{w}}^* = (\tilde{\boldsymbol{X}}^{\mathrm{T}} \tilde{\boldsymbol{X}})^{-1} \tilde{\boldsymbol{X}}^{\mathrm{T}} \boldsymbol{y}$ is the minimizer.

Computational complexity

Bottleneck of computing

$$\tilde{\boldsymbol{w}}^* = \left(\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}}\right)^{-1}\tilde{\boldsymbol{X}}^{\mathrm{T}}\boldsymbol{y}$$

is to invert the matrix $\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}} \in \mathbb{R}^{(\mathsf{D}+1)\times(\mathsf{D}+1)}$

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- there are many faster approaches (such as conjugate gradient)

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- no solution ($\Rightarrow$ RSS has no minimizer? ✗)
- or infinitely many solutions ($\Rightarrow$ infinitely many minimizers ✓)

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sqft	sale price
1000	500K

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Example: $\mathsf{D} = \mathsf{N} = 1$

sqft	sale price
1000	500K

Any line passing this single point is a minimizer of RSS.

How about the following?

$\mathsf{D} = 1, \mathsf{N} = 2$

sqft	sale price
1000	500K
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Any line passing **the average** is a minimizer of RSS.

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Any line passing **the average** is a minimizer of RSS.

$\mathsf{D} = 2, \mathsf{N} = 3$**?**

sqft	#bedroom	sale price
1000	2	500K
1500	3	700K
2000	4	800K

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Any line passing **the average** is a minimizer of RSS.

$D = 2, N = 3$**?**

sqft	#bedroom	sale price
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Again *infinitely many minimizers*.

How to resolve this issue?

Intuition: what does inverting $\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}}$ do?

eigendecomposition: $$\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}} = \boldsymbol{U}^{\mathrm{T}} \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & \lambda_{\mathsf{D}} & 0 \\ 0 & \cdots & 0 & \lambda_{\mathsf{D}+1} \end{bmatrix} \boldsymbol{U}$$

where $\lambda_1 \geq \lambda_2 \geq \cdots \lambda_{\mathsf{D}+1} \geq 0$ are **eigenvalues**.

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inverse:
$$(\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}})^{-1} = \boldsymbol{U}^{\mathrm{T}} \begin{bmatrix} \frac{1}{\lambda_1} & 0 & \cdots & 0 \\ 0 & \frac{1}{\lambda_2} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & \frac{1}{\lambda_{\mathsf{D}}} & 0 \\ 0 & \cdots & 0 & \frac{1}{\lambda_{\mathsf{D}+1}} \end{bmatrix} \boldsymbol{U}$$

i.e. just invert the eigenvalues

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One natural fix: add something positive

$$\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}} + \lambda \boldsymbol{I} = \boldsymbol{U}^{\mathrm{T}} \begin{bmatrix} \lambda_1 + \lambda & 0 & \cdots & 0 \\ 0 & \lambda_2 + \lambda & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & \lambda_{\mathsf{D}} + \lambda & 0 \\ 0 & \cdots & 0 & \lambda_{\mathsf{D}+1} + \lambda \end{bmatrix} \boldsymbol{U}$$

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where $\lambda > 0$ and $\boldsymbol{I}$ is the identity matrix. Now it is invertible:

$$(\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}} + \lambda \boldsymbol{I})^{-1} = \boldsymbol{U}^{\mathrm{T}} \begin{bmatrix} \frac{1}{\lambda_1+\lambda} & 0 & \cdots & 0 \\ 0 & \frac{1}{\lambda_2+\lambda} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & \frac{1}{\lambda_{\mathsf{D}}+\lambda} & 0 \\ 0 & \cdots & 0 & \frac{1}{\lambda_{\mathsf{D}+1}+\lambda} \end{bmatrix} \boldsymbol{U}$$

Fix the problem

The solution becomes

$$\tilde{\boldsymbol{w}}^* = \left(\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}} + \lambda \boldsymbol{I}\right)^{-1} \tilde{\boldsymbol{X}}^{\mathrm{T}}\boldsymbol{y}$$

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- more than an arbitrary hack (as we will see soon)

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λ is a *hyper-parameter*, can be tuned by cross-validation.

Comparison to NNC

Non-parametric versus Parametric

- **Non-parametric methods**: the size of the model *grows* with the size of the training set.
  - e.g. NNC, the training set itself needs to be kept in order to predict. Thus, the size of the model is the size of the training set.

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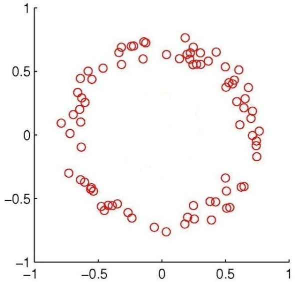
  - e.g. NNC, the training set itself needs to be kept in order to predict. Thus, the size of the model is the size of the training set.
- **Parametric methods**: the size of the model does *not grow* with the size of the training set N.
  - e.g. linear regression, $D + 1$ parameters, independent of N.

Outline

What if linear model is not a good fit?

Example: a straight line is a bad fit for the following data



Solution: nonlinearly transformed features

1. Use a nonlinear mapping

$$\boldsymbol{\phi}(\boldsymbol{x}) : \boldsymbol{x} \in \mathbb{R}^D \rightarrow \boldsymbol{z} \in \mathbb{R}^M$$

to transform the data to a more complicated feature space

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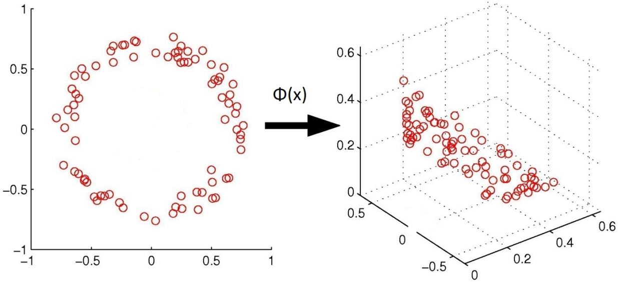

Regression with nonlinear basis

Model: $f(\boldsymbol{x}) = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x})$ where $\boldsymbol{w} \in \mathbb{R}^M$

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Similar least square solution:

$$\boldsymbol{w}^* = \left(\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi}\right)^{-1}\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{y} \quad \text{where} \quad \boldsymbol{\Phi} = \begin{pmatrix} \boldsymbol{\phi}(\boldsymbol{x}_1)^{\mathrm{T}} \\ \boldsymbol{\phi}(\boldsymbol{x}_2)^{\mathrm{T}} \\ \vdots \\ \boldsymbol{\phi}(\boldsymbol{x}_N)^{\mathrm{T}} \end{pmatrix} \in \mathbb{R}^{N \times M}$$

Example

Polynomial basis functions for $D = 1$

$$\boldsymbol{\phi}(x) = \begin{bmatrix} 1 \\ x \\ x^2 \\ \vdots \\ x^M \end{bmatrix} \quad \Rightarrow \quad f(x) = w_0 + \sum_{m=1}^{M} w_m x^m$$

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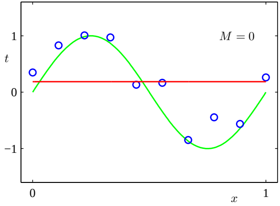
Learning a linear model in the new space
= learning an *M-degree polynomial model* in the original space

Example

Fitting a noisy sine function with a polynomial ($M = 0, 1,$ or 3):



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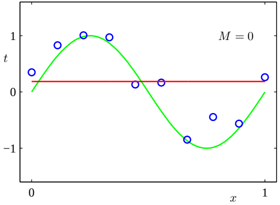

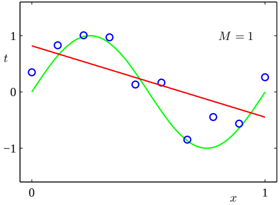

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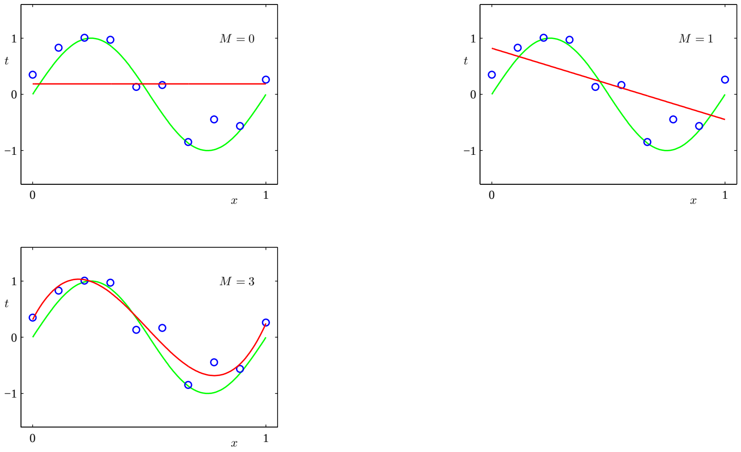

Why nonlinear?

Can I use a fancy **linear feature map**?

$$\boldsymbol{\phi}(\boldsymbol{x}) = \begin{bmatrix} x_1 - x_2 \\ 3x_4 - x_3 \\ 2x_1 + x_4 + x_5 \\ \vdots \end{bmatrix} = \boldsymbol{A}\boldsymbol{x} \quad \text{for some } \boldsymbol{A} \in \mathbb{R}^{\mathsf{M}\times\mathsf{D}}$$

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No, it basically *does nothing* since

$$\min_{\boldsymbol{w}\in\mathbb{R}^{\mathsf{M}}} \sum_n \left(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{A}\boldsymbol{x}_n - y_n\right)^2 = \min_{\boldsymbol{w}'\in\mathrm{Im}(\boldsymbol{A}^{\mathrm{T}})\subset\mathbb{R}^{\mathsf{D}}} \sum_n \left(\boldsymbol{w}'^{\mathrm{T}}\boldsymbol{x}_n - y_n\right)^2$$

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$$\boldsymbol{\phi}(\boldsymbol{x}) = \begin{bmatrix} x_1 - x_2 \\ 3x_4 - x_3 \\ 2x_1 + x_4 + x_5 \\ \vdots \end{bmatrix} = \boldsymbol{A}\boldsymbol{x} \quad \text{for some } \boldsymbol{A} \in \mathbb{R}^{\mathsf{M}\times\mathsf{D}}$$

No, it basically *does nothing* since

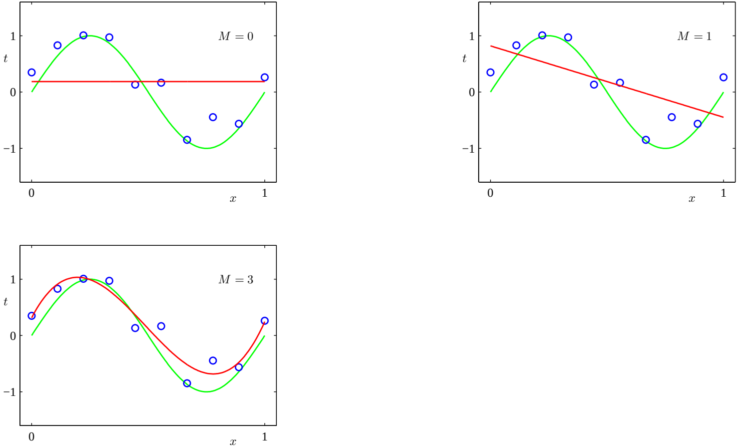
$$\min_{\boldsymbol{w}\in\mathbb{R}^{\mathsf{M}}} \sum_n \left(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{A}\boldsymbol{x}_n - y_n\right)^2 = \min_{\boldsymbol{w}'\in\mathsf{Im}(\boldsymbol{A}^{\mathrm{T}})\subset\mathbb{R}^{\mathsf{D}}} \sum_n \left(\boldsymbol{w}'^{\mathrm{T}}\boldsymbol{x}_n - y_n\right)^2$$

We will see more nonlinear mappings soon.

Outline

Should we use a very complicated mapping?

Ex: fitting a noisy sine function with a polynomial:



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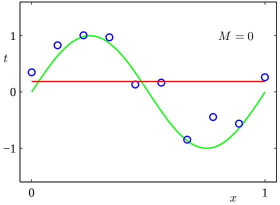

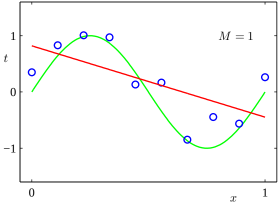

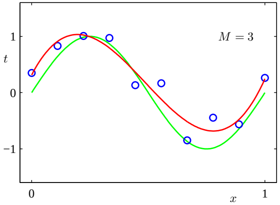

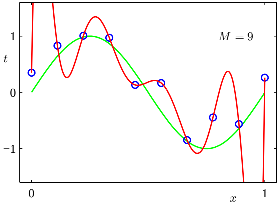

Underfitting and Overfitting

$M \leq 2$ is *underfitting* the data

- large training error
- large test error

$M \geq 9$ is *overfitting* the data

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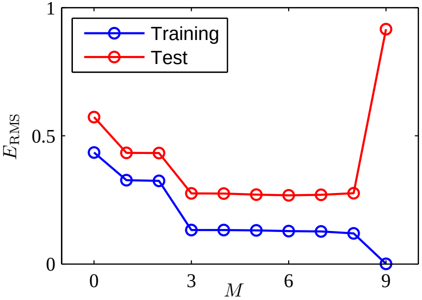

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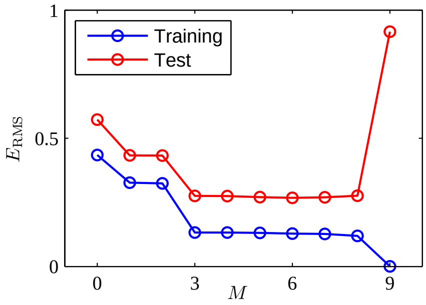

More complicated models ⇒ larger gap between training and test error

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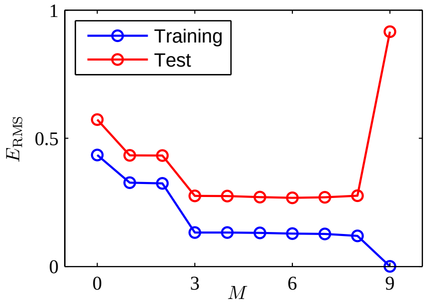

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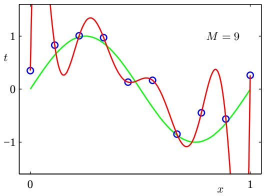
How to prevent overfitting?

Method 1: use more training data

The more, the merrier



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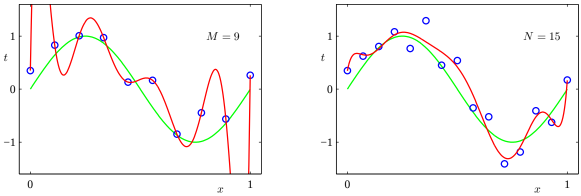

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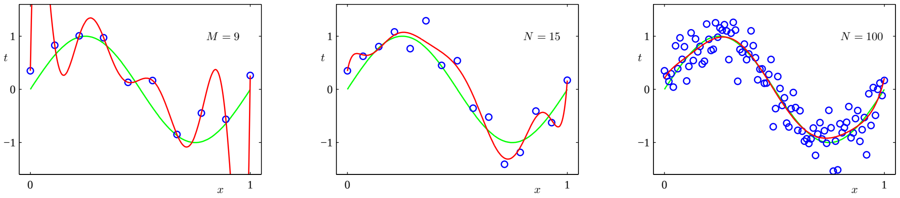

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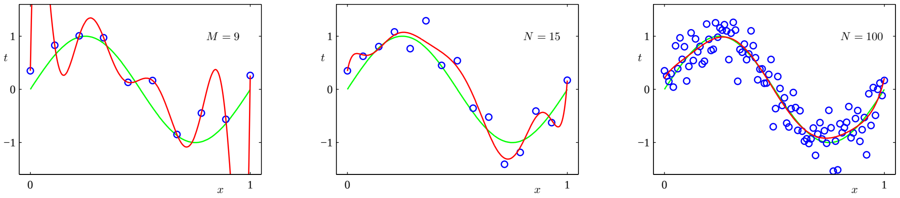

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Method 2: control the model complexity

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- use cross-validation to pick hyper-parameter M

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When M or in general Φ is fixed, are there still other ways to control complexity?

Magnitude of weights

Least square solution for the polynomial example:

	$M = 0$	$M = 1$	$M = 3$	$M = 9$
w_0	0.19	0.82	0.31	0.35
w_1		-1.27	7.99	232.37
w_2			-25.43	-5321.83
w_3			17.37	48568.31
w_4				-231639.30
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Intuitively, **large weights $\Rightarrow$ more complex model**

How to make $\boldsymbol{w}$ small?

Regularized linear regression: new objective

$$\mathcal{E}(\boldsymbol{w}) = \mathrm{RSS}(\boldsymbol{w}) + \lambda R(\boldsymbol{w})$$

Goal: find $\boldsymbol{w}^* = \mathrm{argmin}_w \, \mathcal{E}(\boldsymbol{w})$

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    - measure how complex the model $\boldsymbol{w}$ is, penalize complex models
    - common choices: $\|\boldsymbol{w}\|_2^2$, $\|\boldsymbol{w}\|_1$, etc.
- $\lambda > 0$ is the *regularization coefficient*
    - $\lambda = 0$, no regularization
    - $\lambda \to +\infty$, $\boldsymbol{w} \to \operatorname{argmin}_w R(\boldsymbol{w})$
    - i.e. control **trade-off** between training error and complexity

The effect of λ

when we increase regularization coefficient λ

	$\ln\lambda = -\infty$	$\ln\lambda = -18$	$\ln\lambda = 0$
w_0	0.35	0.35	0.13
w_1	232.37	4.74	-0.05
w_2	-5321.83	-0.77	-0.06
w_3	48568.31	-31.97	-0.06
w_4	-231639.30	-3.89	-0.03
w_5	640042.26	55.28	-0.02
w_6	-1061800.52	41.32	-0.01
w_7	1042400.18	-45.95	-0.00
w_8	-557682.99	-91.53	0.00
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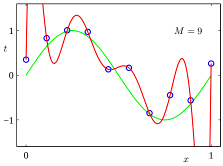
The trade-off

when we increase regularization coefficient λ



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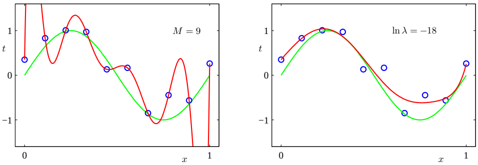

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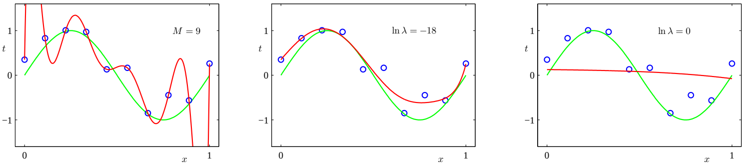

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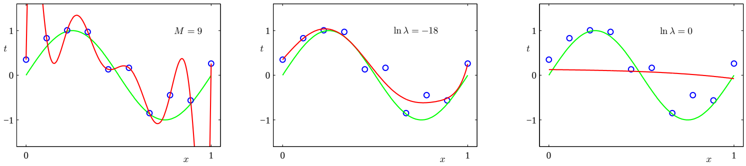

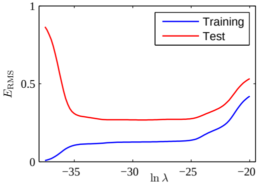

How to solve the new objective?

Simple for $R(\boldsymbol{w}) = \|\boldsymbol{w}\|_2^2$:

$$\mathcal{E}(\boldsymbol{w}) = \mathrm{RSS}(\boldsymbol{w}) + \lambda\|\boldsymbol{w}\|_2^2 = \|\boldsymbol{\Phi}\boldsymbol{w} - \boldsymbol{y}\|_2^2 + \lambda\|\boldsymbol{w}\|_2^2$$

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For other regularizers, as long as it's **convex**, standard optimization algorithms can be applied.

Equivalent form

Regularization is also sometimes formulated as

$$\operatorname*{argmin}_{\boldsymbol{w}} \mathrm{RSS}(w) \quad \textbf{subject to } R(\boldsymbol{w}) \leq \beta$$

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Choosing either λ or β can be done by cross-validation.

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Overfitting: small training error but large test error

Preventing Overfitting: more data + regularization

Recall the question

Typical steps of developing a machine learning system:

- Collect data, split into training, development, and test sets.
- *Train a model with a machine learning algorithm.* Most often we apply cross-validation to tune hyper-parameters.
- Evaluate using the test data and report performance.
- Use the model to predict future/make decisions.

How to do the *red part* exactly?

General idea to derive ML algorithms

1. Pick a set of **models** $\mathcal{F}$
   - e.g. $\mathcal{F} = \{f(\boldsymbol{x}) = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} \mid \boldsymbol{w} \in \mathbb{R}^{\mathsf{D}}\}$
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ML becomes optimization

Outline

Classification

Recall the setup:

- input (feature vector): $\boldsymbol{x} \in \mathbb{R}^{\mathsf{D}}$
- output (label): $y \in [\mathsf{C}] = \{1, 2, \cdots, \mathsf{C}\}$
- goal: learn a mapping $f : \mathbb{R}^{\mathsf{D}} \rightarrow [\mathsf{C}]$

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This lecture: **binary classification**

- Number of classes: $\mathsf{C} = 2$
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We have discussed **nearest neighbor classifier**:

- require carrying the training set
- more like a heuristic

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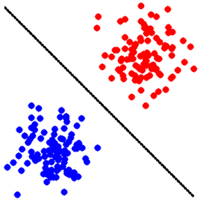

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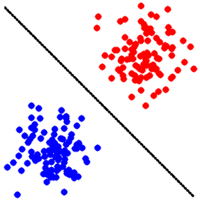
Sign of $\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$ predicts the label:

$$\text{sign}(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}) = \begin{cases} +1 & \text{if } \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} > 0 \\ -1 & \text{if } \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} \leq 0 \end{cases}$$

(Sometimes use sgn for sign too.)



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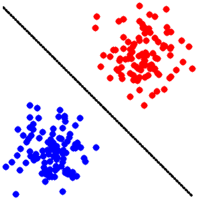

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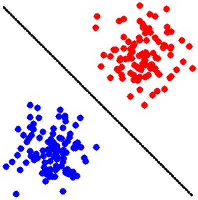
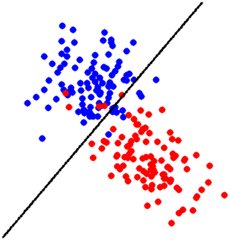


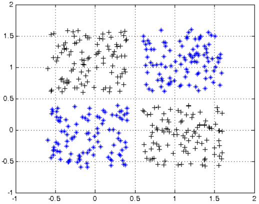
The models

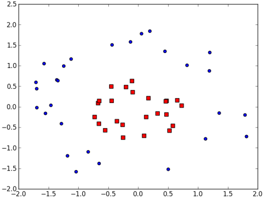
Still makes sense for “almost” linearly separable data



The models

For clearly not linearly separable data,





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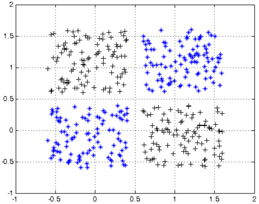

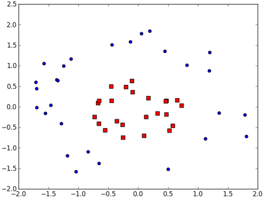

Again can apply a **nonlinear mapping** $\boldsymbol{\Phi}$:

$$\mathcal{F} = \{f(\boldsymbol{x}) = \mathsf{sgn}(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\Phi}(\boldsymbol{x})) \mid \boldsymbol{w} \in \mathbb{R}^{\mathsf{M}}\}$$

More discussions in the next two lectures.

0-1 Loss

Step 2. Define error/loss $L(y', y)$.

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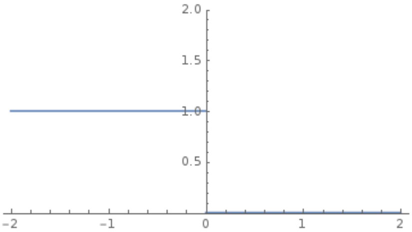
Most natural one for classification: **0-1 loss** $L(y', y) = \mathbb{I}[y' \neq y]$

For classification, more convenient to look at the loss **as a function of** $\boldsymbol{y\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}}$. That is, with

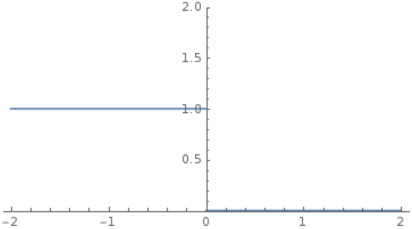
$$\ell_{\text{0-1}}(z) = \mathbb{I}[z \leq 0]$$



the loss for hyperplane $\boldsymbol{w}$ on example $(\boldsymbol{x}, y)$ is $\ell_{\text{0-1}}(y\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x})$

Minimizing 0-1 loss is hard

However, 0-1 loss is *not convex*.



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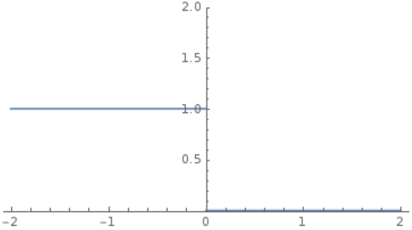
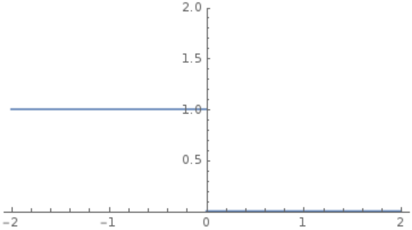


Even worse, minimizing 0-1 loss is *NP-hard in general*.

Surrogate Losses

Solution: find a **convex surrogate loss**



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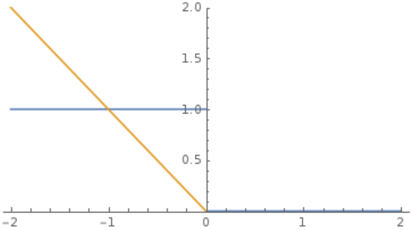

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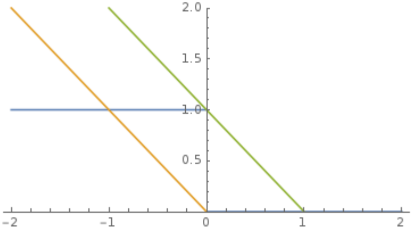

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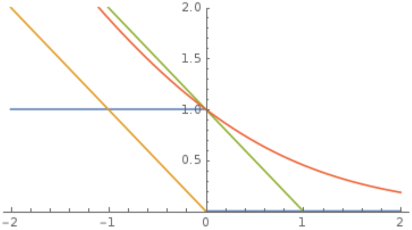

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- logistic loss $\ell_{\text{logistic}}(z) = \log(1 + \exp(-z))$ (used in logistic regression; the base of $\log$ doesn't matter)

ML becomes convex optimization

Step 3. Find ERM:

$$\boldsymbol{w}^* = \underset{\boldsymbol{w}\in\mathbb{R}^{\mathsf{D}}}{\operatorname{argmin}} \sum_{n=1}^{N} \ell(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n) = \underset{\boldsymbol{w}\in\mathbb{R}^{\mathsf{D}}}{\operatorname{argmin}} \frac{1}{N} \sum_{n=1}^{N} \ell(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n)$$

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Datasets

Training data

- N samples/instances: $\mathcal{D}^{\text{TRAIN}} = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \cdots, (\boldsymbol{x}_{\mathsf{N}}, y_{\mathsf{N}})\}$
- They are used to learn $f(\cdot)$

Test data

- M samples/instances: $\mathcal{D}^{\text{TEST}} = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \cdots, (\boldsymbol{x}_{\mathsf{M}}, y_{\mathsf{M}})\}$
- They are used to evaluate how well $f(\cdot)$ will do.

Development/Validation data

- L samples/instances: $\mathcal{D}^{\text{DEV}} = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \cdots, (\boldsymbol{x}_{\mathsf{L}}, y_{\mathsf{L}})\}$
- They are used to optimize hyper-parameter(s).

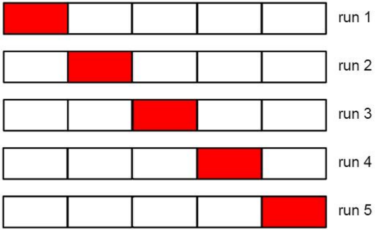
These three sets should *not* overlap!

S-fold Cross-validation

What if we do not have a development set?

- Split the training data into S equal parts.
- Use each part *in turn* as a development dataset and use the others as a training dataset.
- Choose the hyper-parameter leading to best *average* performance.

$\mathrm{S} = 5$: 5-fold cross validation



Special case: $\mathrm{S} = \mathrm{N}$, called leave-one-out.

High level picture

Typical steps of developing a machine learning system:

- Collect data, split into training, development, and test sets.
- *Train a model with a machine learning algorithm.* Most often we apply cross-validation to tune hyper-parameters.
- Evaluate using the test data and report performance.
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Outline

Numerical optimization

Problem setup

- Given: a function $F(\boldsymbol{w})$
- Goal: minimize $F(\boldsymbol{w})$ (approximately)

First-order optimization methods

Two simple yet extremely popular methods

- **Gradient Descent (GD)**: simple and fundamental
- **Stochastic Gradient Descent (SGD)**: faster, effective for large-scale problems

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Gradient is sometimes referred to as *first-order* information of a function. Therefore, these methods are called *first-order methods*.

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GD: keep moving in the *negative gradient direction*

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- might need to be **changing** over iterations (think $F(w) = |w|$)
- adaptive and automatic step size tuning is an active research area

An example

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- until $F(\boldsymbol{w}^{(t)})$ **does not change much** or t **reaches a fixed number**

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Intuition: by first-order **Taylor approximation**

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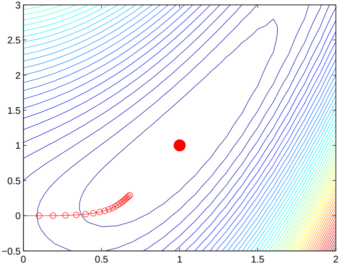

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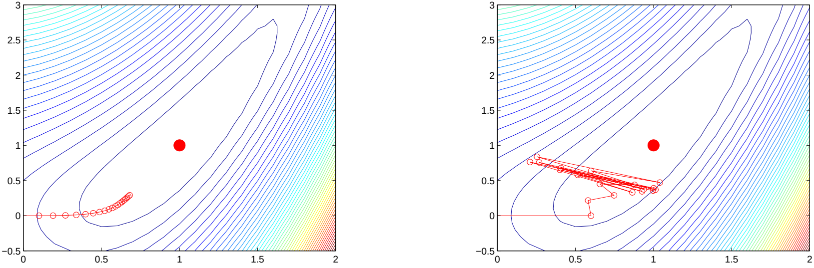

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but large η is unstable

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Key point: it could be *much faster to obtain a stochastic gradient!*
(examples coming soon)

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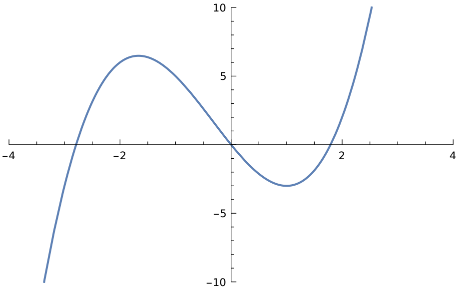
- for nonconvex objectives, *what does it mean?*

Convergence guarantees — nonconvex objectives

A stationary point can be a **local minimizer**



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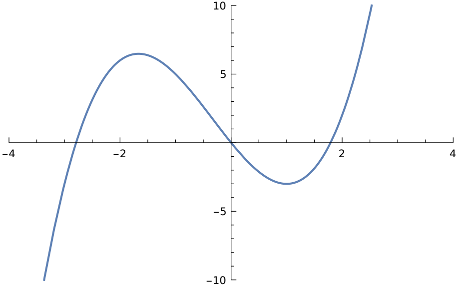

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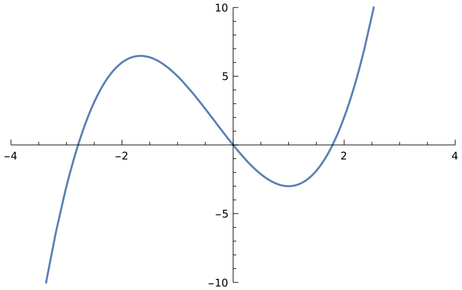

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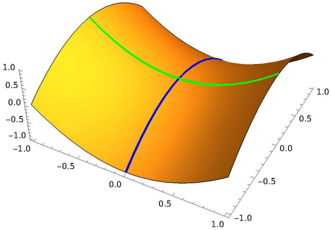

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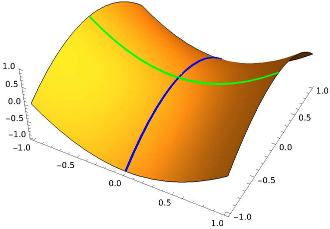

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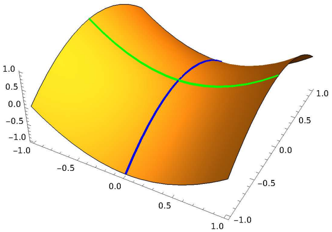

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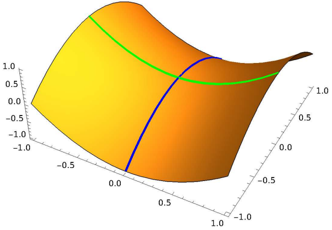

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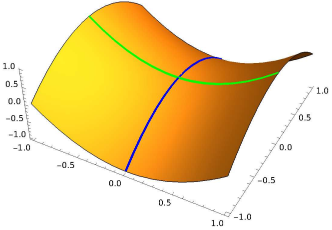

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Convergence guarantees — nonconvex objectives

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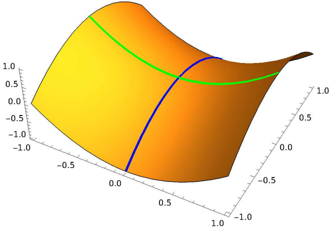

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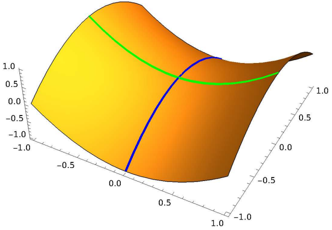

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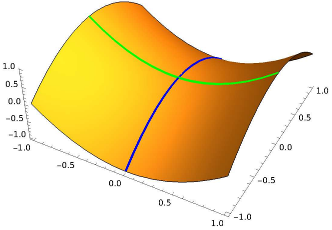

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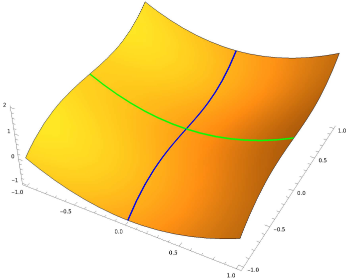

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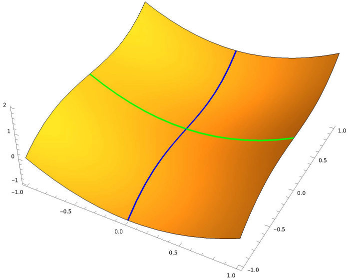

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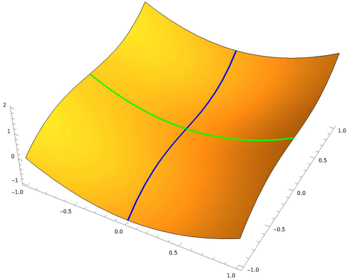

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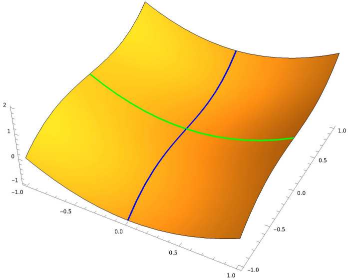

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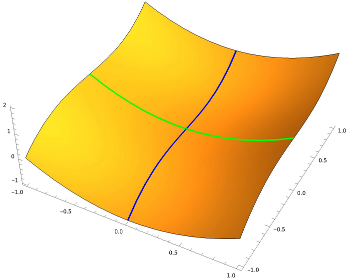

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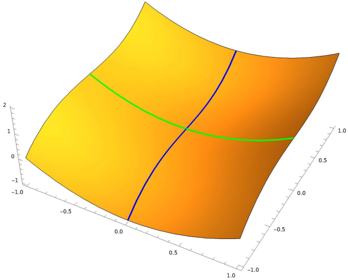

Even worse, distinguishing local min and saddle point is generally *NP-hard*.

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- recent research shows that *many problems have no "bad" saddle points or even "bad" local minimizers*
- justify the practical effectiveness of GD/SGD (default method to try)

Second-order methods

Recall the intuition of GD: we look at first-order **Taylor approximation**

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where $\boldsymbol{H}_t = \nabla^2 F(\boldsymbol{w}^{(t)}) \in \mathbb{R}^{\mathsf{D}\times\mathsf{D}}$ is the *Hessian* of F at $\boldsymbol{w}^{(t)}$, i.e.,

$$H_{t,ij} = \frac{\partial^2 F(\boldsymbol{w})}{\partial w_i \partial w_j}\Big|_{\boldsymbol{w}=\boldsymbol{w}^{(t)}}$$

(think "second derivative" when $D = 1$)

Newton method

If we minimize the second-order approximation (via "complete the square")

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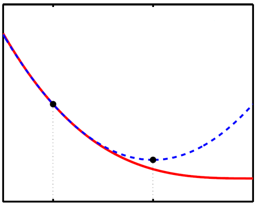

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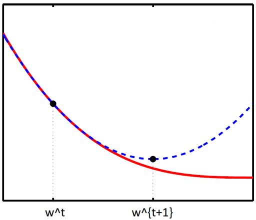
for convex F (so H_t is *positive semidefinite*)
we obtain **Newton method**:

$$\boldsymbol{w}^{(t+1)} \leftarrow \boldsymbol{w}^{(t)} - \boldsymbol{H}_t^{-1}\nabla F(\boldsymbol{w}^{(t)})$$



Comparing GD and Newton

$$\boldsymbol{w}^{(t+1)} \leftarrow \boldsymbol{w}^{(t)} - \eta \nabla F(\boldsymbol{w}^{(t)}) \quad \text{(GD)}$$

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- computing Hessian in each iteration is *very slow* though
- does not really make sense for *nonconvex objectives* (but generally Hessian can be useful for escaping saddle points)

Outline

Recall the perceptron loss

$$F(\boldsymbol{w}) = \frac{1}{N}\sum_{n=1}^{N} \ell_{\textsf{perceptron}}(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n)$$
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Let's approximately minimize it with GD/SGD.

Applying GD to perceptron loss

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Slow: each update makes one pass of the entire training set!

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One common trick: pick one example $n \in [N]$ uniformly at random, let

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Conveniently, objective of most ML tasks is a *finite sum* (over each training point) and the above trick applies!

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- why $\eta = 1$? Does not really matter in terms of prediction of $\boldsymbol{w}$

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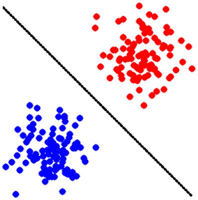
Thus it is more likely to get it right after the update.

Any theory?

(HW 1) If training set is linearly separable

- Perceptron *converges in a finite number of steps*
- training error is 0



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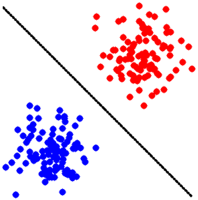

There are also guarantees when the data are not linearly separable.

Outline

A simple view

In one sentence: find the minimizer of

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Before optimizing it: *why logistic loss? and why "regression"?*

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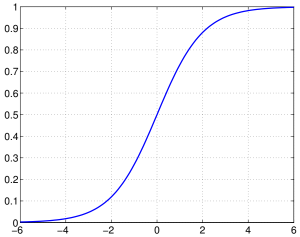
One way: **sigmoid function + linear model**

$$\mathbb{P}(y = +1 \mid \boldsymbol{x}; \boldsymbol{w}) = \sigma(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x})$$

where σ is the sigmoid function:

$$\sigma(z) = \frac{1}{1 + e^{-z}}$$



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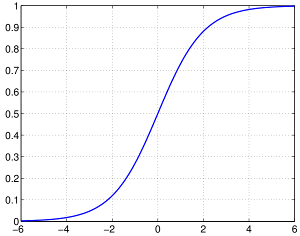

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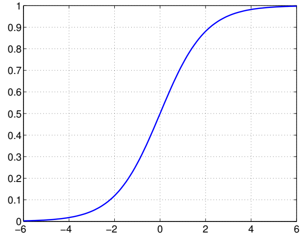

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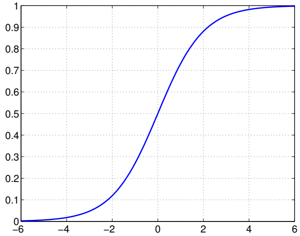

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Properties of sigmoid $\sigma(z) = \frac{1}{1+e^{-z}}$

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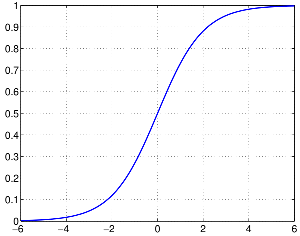

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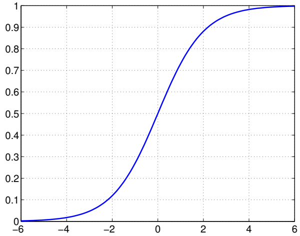

The probability of label -1 is naturally

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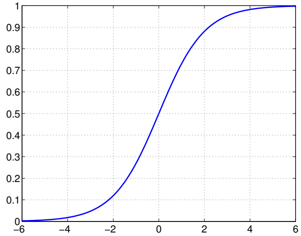

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and thus

$$\mathbb{P}(y \mid \boldsymbol{x}; \boldsymbol{w}) = \sigma(y\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}) = \frac{1}{1 + e^{-y\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}}}$$

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What we observe are labels, not probabilities.

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- perform Maximum Likelihood Estimation (MLE)

Specifically, what is the probability of seeing label $y_1, \cdots, y_n$ given $x_1, \cdots, x_n$, as a function of some $\boldsymbol{w}$?

$$P(\boldsymbol{w}) = \prod_{n=1}^{N} \mathbb{P}(y_n \mid \boldsymbol{x_n}; \boldsymbol{w})$$

MLE: find $\boldsymbol{w}^*$ that **maximizes the probability** $P(\boldsymbol{w})$

The MLE solution

$$\boldsymbol{w}^* = \underset{\boldsymbol{w}}{\operatorname{argmax}}\, P(\boldsymbol{w}) = \underset{\boldsymbol{w}}{\operatorname{argmax}} \prod_{n=1}^{N} \mathbb{P}(y_n \mid \boldsymbol{x_n}; \boldsymbol{w})$$

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&= \operatorname*{argmin}_{\boldsymbol{w}} F(\boldsymbol{w})
\end{aligned}
$$

i.e. *minimizing logistic loss is exactly doing MLE for the sigmoid model!*

Let's apply SGD again

$$\boldsymbol{w} \leftarrow \boldsymbol{w} - \eta \tilde{\nabla} F(\boldsymbol{w})$$

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$$\begin{aligned} \boldsymbol{w} &\leftarrow \boldsymbol{w} - \eta\tilde{\nabla}F(\boldsymbol{w}) \\ &= \boldsymbol{w} - \eta\nabla_{\boldsymbol{w}}\ell_{\text{logistic}}(y_n\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n) \qquad (n \in [N] \text{ is drawn u.a.r.}) \end{aligned}$$

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&= \boldsymbol{w} + \eta \mathbb{P}(-y_n \mid \boldsymbol{x}_n; \boldsymbol{w}) y_n \boldsymbol{x}_n
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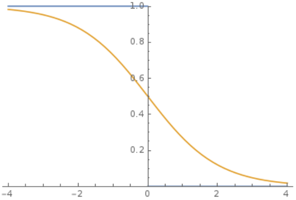
&= \boldsymbol{w} + \eta\mathbb{P}(-y_n \mid \boldsymbol{x}_n;\boldsymbol{w})y_n\boldsymbol{x}_n
\end{aligned}$$

This is a *soft version of Perceptron!*

$\mathbb{P}(-y_n|\boldsymbol{x}_n;\boldsymbol{w})$ versus $\mathbb{I}[y_n \neq \text{sgn}(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n)]$



Applying Newton to logistic loss

$$\nabla_{\boldsymbol{w}} \ell_{\text{logistic}}(y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n) = -\sigma(-y_n \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n) y_n \boldsymbol{x}_n$$

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Exercises:

- why is the Hessian of logistic loss positive semidefinite?

Applying Newton to logistic loss

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Exercises:

- why is the Hessian of logistic loss positive semidefinite?
- can we apply Newton method to perceptron/hinge loss?