Yandex

SCHOOL OF DATA ANALYSIS

Skoltech

Skolkovo Institute of Science and Technology

МИСиС

Intro into Machine Learning

Linear Models. Numerical optimization. Logistic Regression. Figures of Merits. Overfitting. Model Selection. Regularization.

Advanced Computing and Machine Learning Course
25-27 May 2020, IGFAE

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Lecture overview

- Linear models for regression
- Numerical and stochastic optimization at a glance
- Linear models for classification
- Figures of merits
- Overfitting: how to fool the linear regression
- Regularization

“Physics-based” vs. machine-learned models

› Some criteria for machine learning to be applied in a dependency recovery setting:

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  - The dependency has a complex form too hard for manual examination
  - A sample from the dependency of sufficiently large size is available

“Physics-based” vs. machine-learned models

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Machine learning as function approximation

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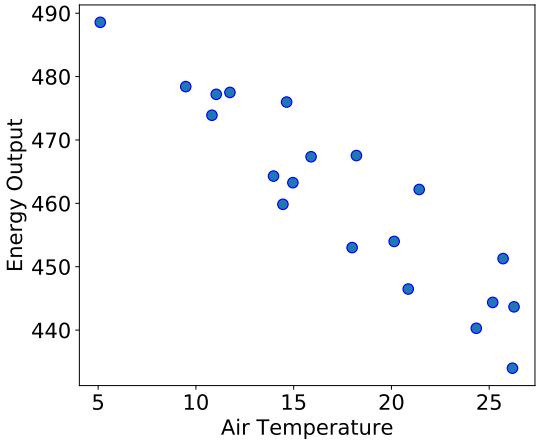
- Learning: the search for the optimal hypothesis $h \in \mathbb{H}$ w. r. t. the fixed loss function

Function approximation: energy usage



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Function approximation: energy usage

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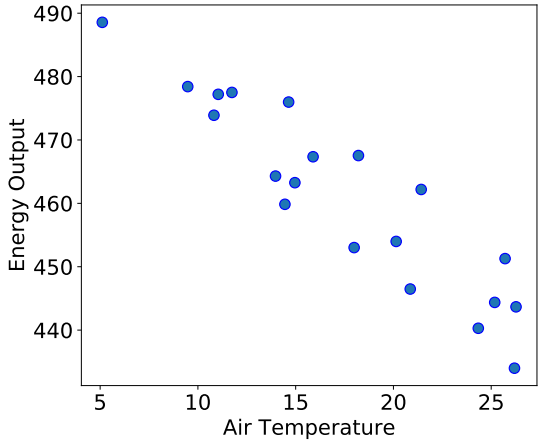

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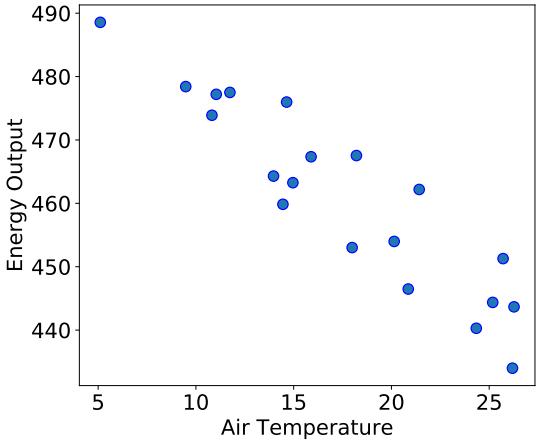

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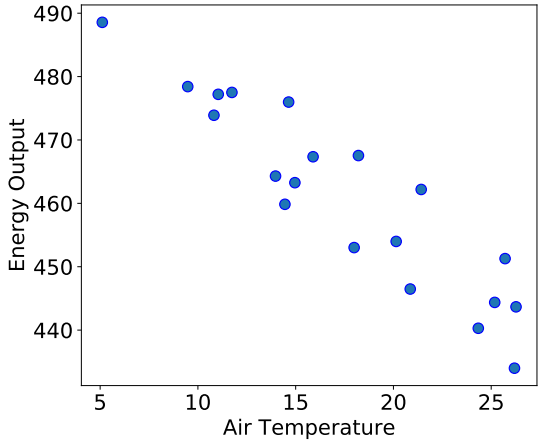

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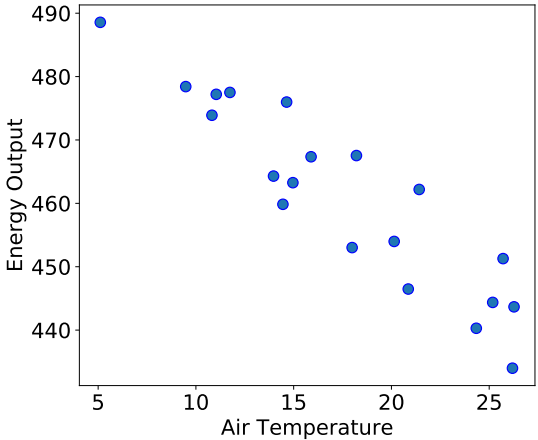

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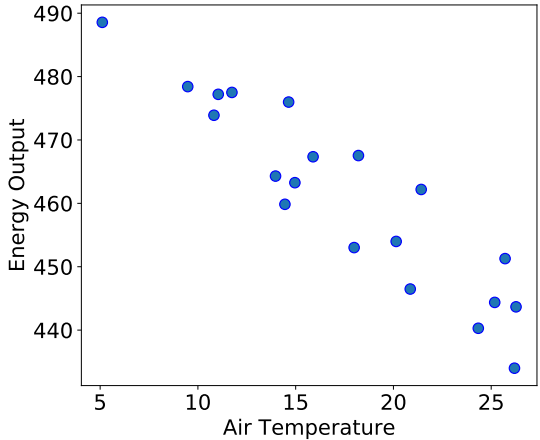

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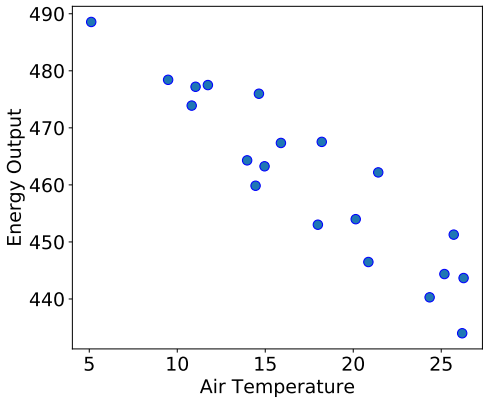
Linear models for regression

Univariate linear regression

› A single feature (regressor) x:
Air Temperature



Univariate linear regression

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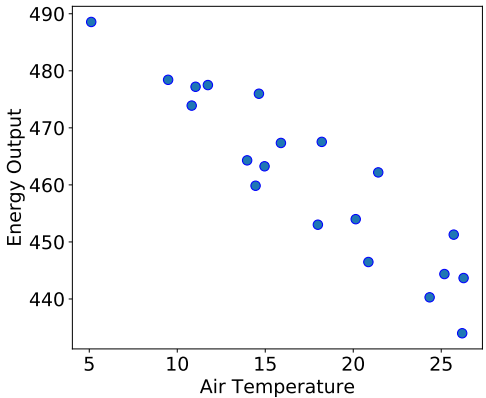

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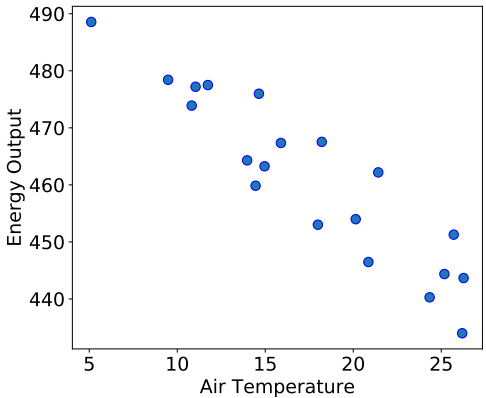

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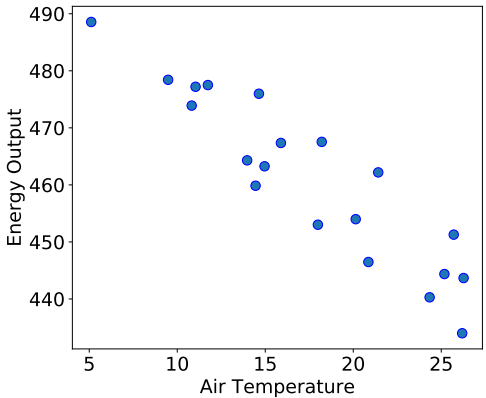

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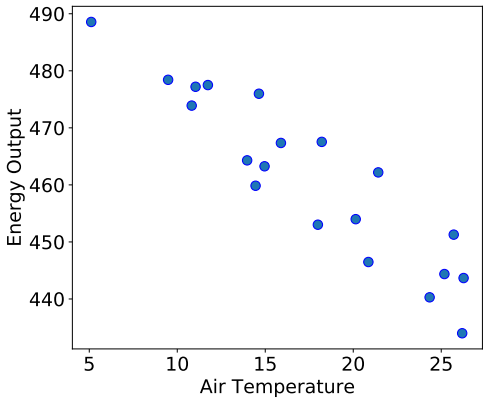

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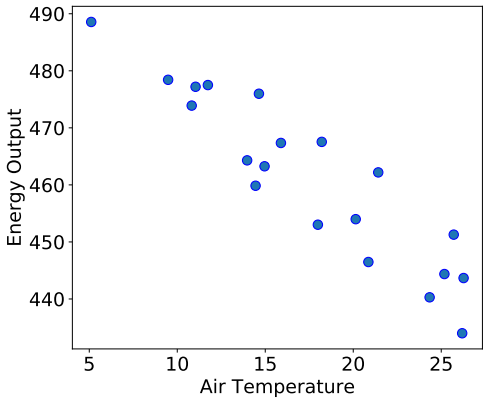
- The goal: given X^ℓ, find $\mathbf{w} = (w_1, w_0)$



Univariate linear regression

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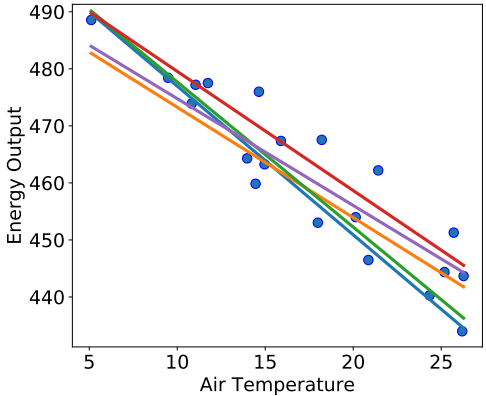
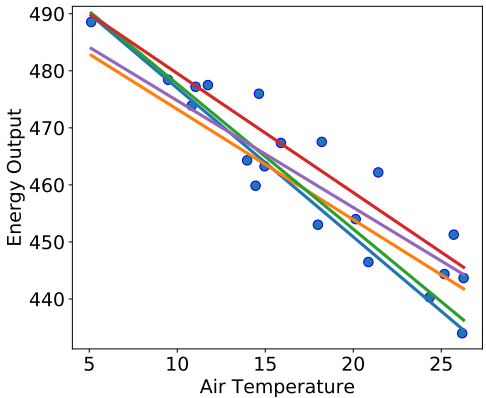


Univariate linear regression

- Which fit to choose?
- With the linear model being fixed, depends on the data and the loss function!



Univariate linear regression

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- Mean square (L2) loss (MSE):

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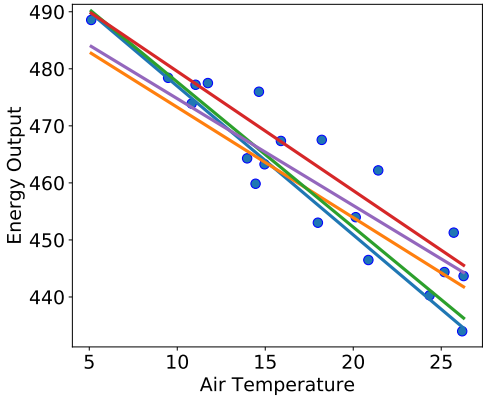

Some other evaluation metrics for regression

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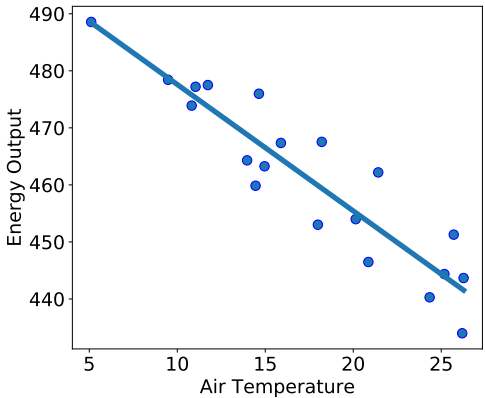
- Mean absolute error: $\mathrm{MAE}(h, X^\ell) = \frac{1}{\ell}\sum_{i=1}^{\ell}|y_i - h(x_i)|$

Univariate linear regression

› With the loss fixed, the linear problem reduces to optimization:

$$\frac{1}{\ell}\sum_{i=1}^{\ell}(y_i - w_1 x_i - w_0)^2 \to \min_{(w_0,w_1)\in\mathbb{R}^2},$$



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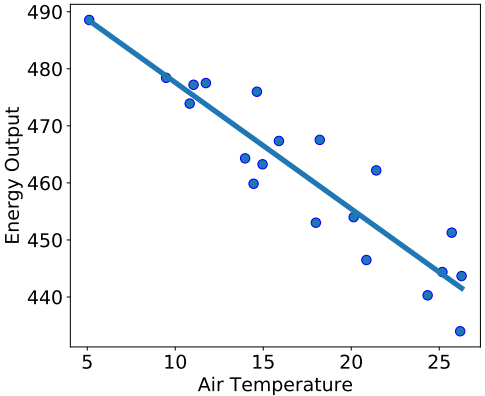
to which an analytical solution is available

$$\widehat{w}_1 = \frac{\sum_{i=1}^{\ell}(x_i - \mu_x)(y_i - \mu_y)}{\sum_{i=1}^{\ell}(x_i - \mu_x)^2},$$

$$\widehat{w}_0 = \mu_y - \widehat{w}_1\mu_x$$

with $\mu_x = \frac{1}{\ell}\sum_{i=1}^{\ell} x_i, \quad \mu_y = \frac{1}{\ell}\sum_{i=1}^{\ell} y_i$



Multivariate linear regression

- Multiple features (regressors) $\mathbf{x}_i = (x_{1i}, \dots x_{di})$ available for each y_i
- The model:

$$
\begin{aligned}
y_1 &= w_1 x_{11} + \dots w_d x_{d1} + \varepsilon_1, \\
y_2 &= w_1 x_{12} + \dots w_d x_{d2} + \varepsilon_2, \\
&\dots \\
y_\ell &= w_1 x_{1\ell} + \dots w_d x_{d\ell} + \varepsilon_\ell,
\end{aligned}
$$

is often written in matrix-vector form as

$$
\begin{bmatrix} y_1 \\ \vdots \\ y_\ell \end{bmatrix} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{d1} \\ \vdots & \vdots & \ddots & \vdots \\ x_{1\ell} & x_{2\ell} & \dots & x_{d\ell} \end{bmatrix} \begin{bmatrix} w_1 \\ \vdots \\ w_d \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_\ell \end{bmatrix} \quad \longleftrightarrow \quad \boldsymbol{y} = \boldsymbol{X}\mathbf{w} + \boldsymbol{\varepsilon}
$$

Multivariate linear regression: the solution

› The problem: minimize MSE

$$Q(h, X^l) = \sum_{i=1}^{\ell} \Big(y_i - \sum_{k=1}^{d} w_k x_{ki}\Big)^2 \equiv \|\boldsymbol{y} - \boldsymbol{X}\mathbf{w}\|^2 \to \min_{\mathbf{w}\in\mathbb{R}^d}$$

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$$\nabla_{\mathbf{w}} \|\boldsymbol{y} - \boldsymbol{X}\mathbf{w}\|^2 = 2(\boldsymbol{y} - \boldsymbol{X}\mathbf{w})\boldsymbol{X} = 0$$

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- The solution

$$\mathbf{w}^* = (\boldsymbol{X}^\intercal \boldsymbol{X})^{-1} \boldsymbol{X}^\intercal \boldsymbol{y}$$

Numerical and stochastic optimization at a glance

A quick intro into the Numerical Optimization

› Consider the optimization problem in $\mathbb{R}^d$

$$f(\mathbf{x}) \to \min_{\mathbf{x} \in \mathbb{R}^d}$$

(such as $f(\mathbf{w}) \equiv \sum_{i=1}^{\ell} \left(y_i - \sum_{k=1}^{d} w_k x_{ki} \right)^2 \to \min_{\mathbf{w} \in \mathbb{R}^d}$)

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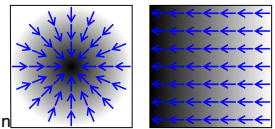
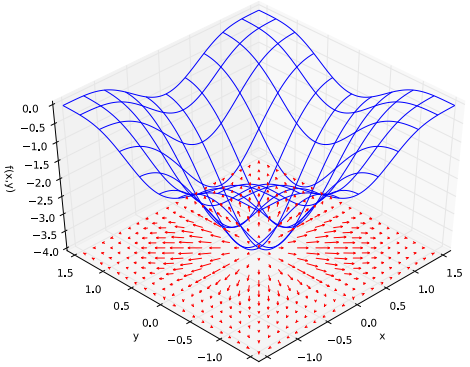
› In general, solved using the numerical methods such as the gradient descent

› Gradients: directions in $\mathbb{R}^d$ pointing towards steepest function increase

$$\nabla_{\mathbf{x}} f(\mathbf{x}) \equiv \left(\frac{\partial f(\mathbf{x})}{\partial x_1}, \ldots, \frac{\partial f(\mathbf{x})}{\partial x_d}\right)$$





The gradient descent algorithm

› The gradient descent procedure iterates from $\mathbf{x}^{(0)}$ as

$$\mathbf{x}^{(k)} \leftarrow \mathbf{x}^{(k-1)} - \alpha_k \nabla_{\mathbf{x}} f(\mathbf{x}^{(k-1)})$$

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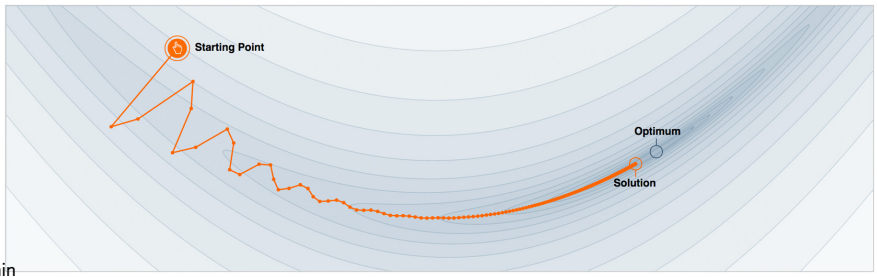
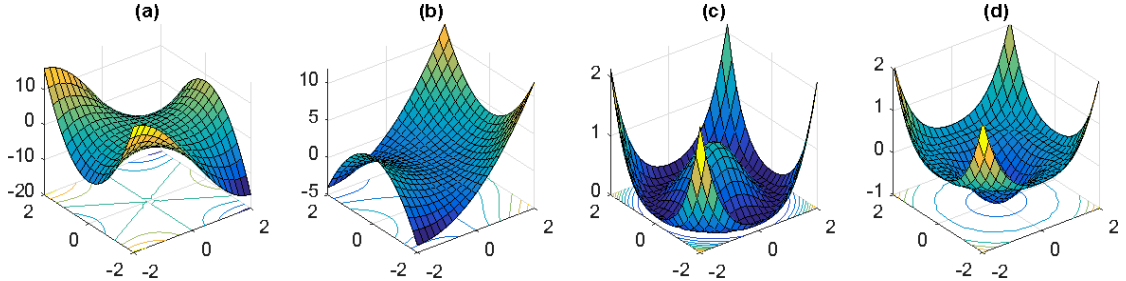
› For smooth convex functions with a single minimum $\mathbf{x}^*$, k steps of gradient descent achieve accuracy $f(\mathbf{x}^{(k)}) - f(\mathbf{x}^*) = \mathcal{O}(1/k)$



The gradient descent with non-convex targets



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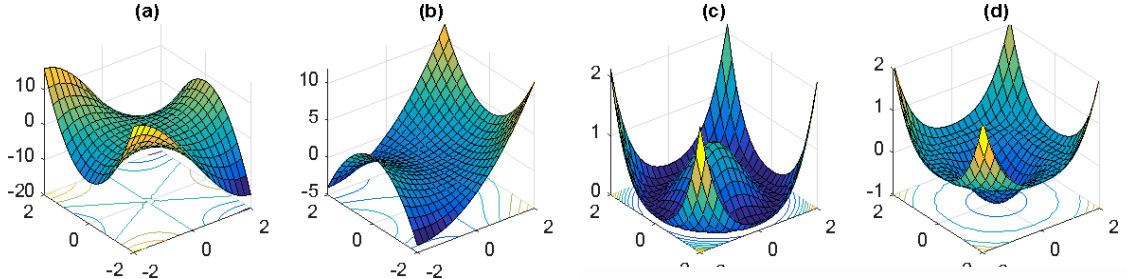
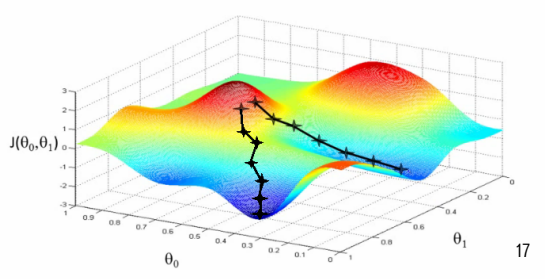


› Trajectories of gradient descent over non-convex functions may (and will) not always end up in a single optimum



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- Use subsamples for gradient estimation: the Stochastic Gradient Descent (SGD)
  1. Pick $i_k \in \{1, \ldots, \ell\}$ at random;
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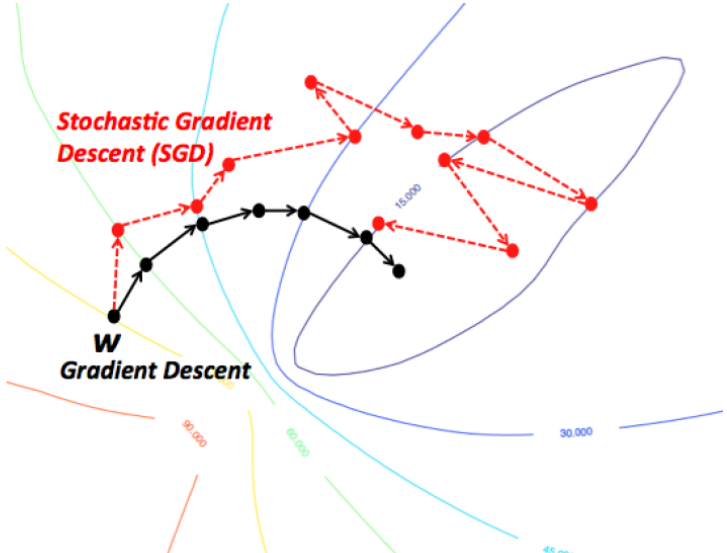
- Machine learning: many additive targets $f(\mathbf{w}) = \sum_{i=1}^{\ell} f_i(\mathbf{w})$, computationally inefficient for large ℓ
- Use subsamples for gradient estimation: the Stochastic Gradient Descent (SGD)
  1. Pick $i_k \in \{1, \ldots, \ell\}$ at random;
  2. Compute $\mathbf{w}^{(k)} \leftarrow \mathbf{w}^{(k-1)} - \alpha_k \nabla_{\mathbf{w}} f_{i_k}(\mathbf{w}^{(k-1)})$
- For smooth convex functions with a single minimum $\mathbf{x}^*$, k steps of SGD achieve accuracy $f(\mathbf{w}^{(k)}) - f(\mathbf{w}^*) = \mathcal{O}(1/\sqrt{k})$
- Batching, variance reduction, momentum hacks available to improve the convergence rate to $\mathcal{O}(1/k)$

Gradient descent VS stochastic gradient descent

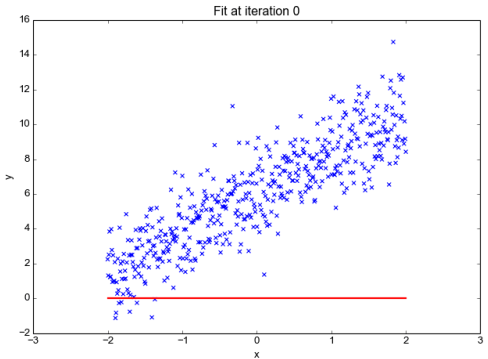


An example: SGD for multivariate linear regression

- Initialize with some $\mathbf{w}^{(0)}$
- Gradient in i_kth object is

$$\nabla_{\mathbf{x}} f_{i_k}(\mathbf{w}) = 2(y_{i_k} - \mathbf{x}_{i_k}^{\mathsf{T}}\mathbf{w})\mathbf{x}_{i_k} \qquad (\in \mathbb{R}^d)$$

- Compute updates using SGD:
$\mathbf{w}^{(k)} \leftarrow \mathbf{w}^{(k-1)} - \alpha_k \nabla_{\mathbf{w}} f_{i_k}(\mathbf{w}^{(k-1)})$



Linear models for classification

Binary classification

- An unknown distribution D generates instances $(\mathbf{x}_1, \mathbf{x}_2, \ldots)$

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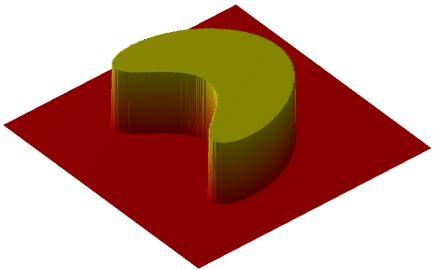

There exist sets A^+, A^- such that $A^+ \equiv \{i : \mathbf{x}_i \in D : y_i = +1\}$ and $A^- \equiv \{i : \mathbf{x}_i \in D : y_i = -1\}$ with indicator functions $\chi_{A^+}(\cdot), \chi_{A^-}(\cdot)$ (displayed on the left)

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- The error of the classifier h is the probability (over D) that it will fail

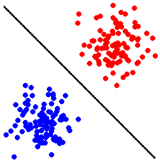
$$Q(h, D) = \Pr_{\mathbf{x} \sim D}[f(\mathbf{x}) \neq h(\mathbf{x})]$$

usually estimated by the accuracy metric

$$Q(h, X^\ell) = \frac{1}{\ell} \sum_{i=1}^{\ell} [f(\mathbf{x}_i) \neq h(\mathbf{x}_i)]$$

Linear models for classification

› Linear model: $h(\mathbf{x}) = \text{sign}\Big(\sum_{i=1}^{d} w_i x_i + w_0\Big) = \text{sign}\big(\mathbf{w}^\intercal \mathbf{x} + w_0\big)$



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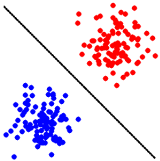

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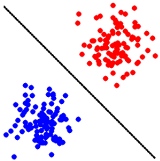

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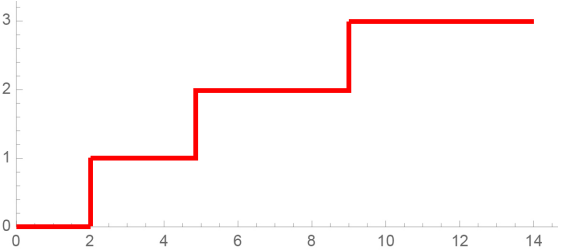
(cannot optimize using gradient descent)



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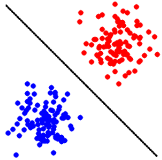

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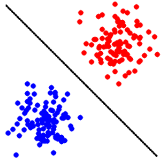

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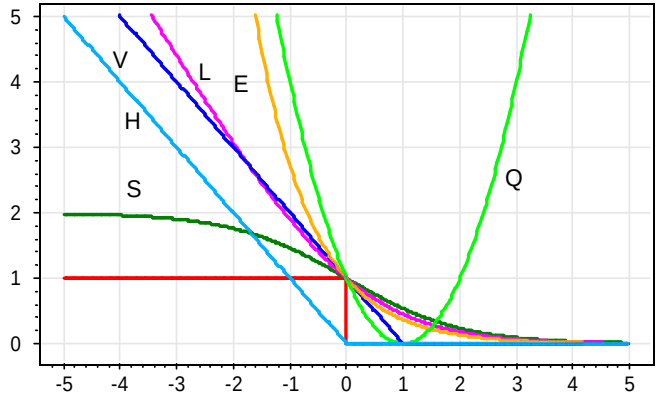
- $Q(h, X^\ell)$ can be written using $Q(h, X^\ell) = \frac{1}{\ell} \sum_{i=1}^{\ell} L(M_i)$
  where $L(M_i) = [M_i < 0] \equiv [y_i \mathbf{w}^\intercal \mathbf{x}_i < 0]$
- Upper-bounding $L(M)$ yields upper bounds for $Q(h, X^\ell)$

Linear models for classification: upper bounds

Multiple approximations to accuracy

- $L_{\mathsf{L}}(M) = \log(1 + e^{-M})$
- $L_{\mathsf{H}}(M) = \max(0, 1 - M)$
- $L_{\mathsf{P}}(M) = \max(0, -M)$
- $L_{\mathsf{E}}(M) = e^{-M}$
- $L_{\mathsf{S}}(M) = 2/(1 + e^{M})$

and their respective optimization procedures give rise to various learning algorithms



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is often written via log-likelihood (of which the negative is log-loss)

$$\log L(X^\ell) = \sum_{i=1}^{\ell} [y_i = +1] \log h(\mathbf{x}_i) + [y_i = -1] \log(1 - h(\mathbf{x}_i))$$

The logistic regression model

- The choice of h: sigmoid function

$$h(\mathbf{x}) = \sigma(\mathbf{w}^\mathsf{T}\mathbf{x})$$

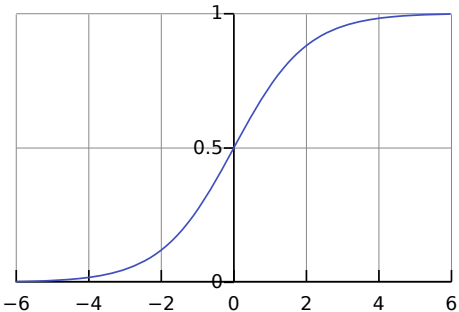
where $\sigma(x) \in [0, 1]$

- Typical choice: the logistic function

$$\sigma(\mathbf{w}^\mathsf{T}\mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^\mathsf{T}\mathbf{x})}$$

- Plugging the logistic function into the loss yields an approximation of accuracy

$$\sum_{i=1}^{\ell}(1 + \exp(\mathbf{w}^\mathsf{T}\mathbf{x})) \to \min_{\mathbf{w}\in\mathbb{R}^d}$$



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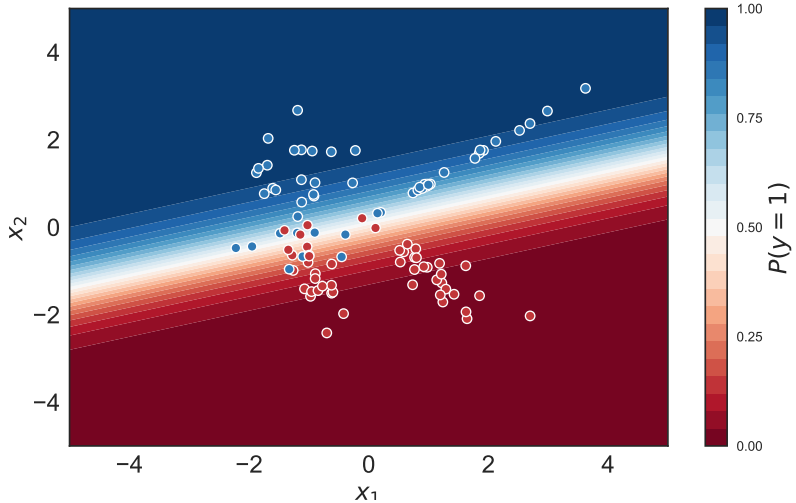

Figures of merits

Classification quality evaluation: accuracy

› Given a labeled sample $X^\ell = \left\{(\mathbf{x}_i, y_i)\right\}_{i=1}^{\ell}$, $y_i \in \{-1, +1\}$, and some candidate h, how well does h perform on X^ℓ?

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- Obvious choice: accuracy

$$\text{accuracy}(a, X^\ell) = \frac{1}{\ell}\sum_{i=1}^{\ell}[a(\mathbf{x}_i) = y_i]$$

- Example: Higgs challenge — selection of the interesting signal $H \to \tau\tau$ decay against the already known backround
- 164,333 background, 85,667 signal events (66% background)

Classification quality evaluation: confusion matrix

	Label $y = 1$	Label $y = -1$
Decision $a(x) = 1$	True Positive (TP)	False Positive (FP)
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› While accuracy can be expressed, too

$$\text{accuracy} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{FP} + \text{FN} + \text{TN}}$$

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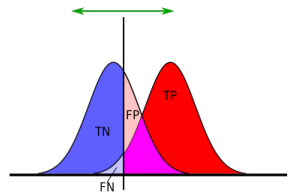
- Area under curve (ROC-AUC) reflects classification quality



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- Criteria better suited for imbalanced problems:

$$\text{precision} = \frac{\text{TP}}{\text{TP} + \text{FP}}, \qquad \text{recall} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

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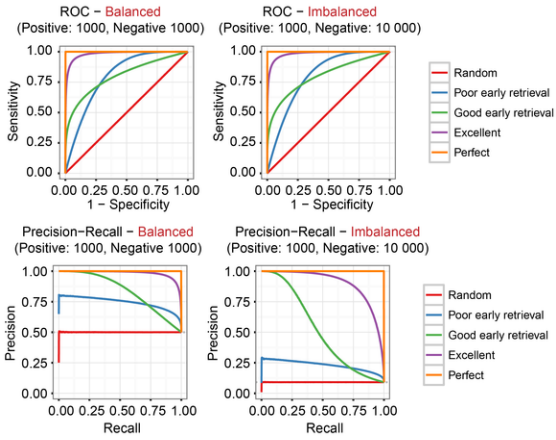

Source: classeval.wordpress.com

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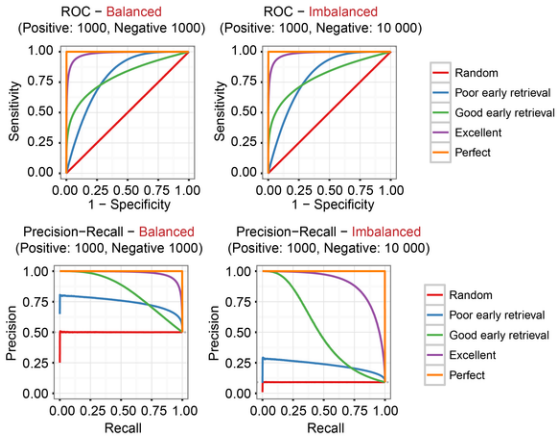

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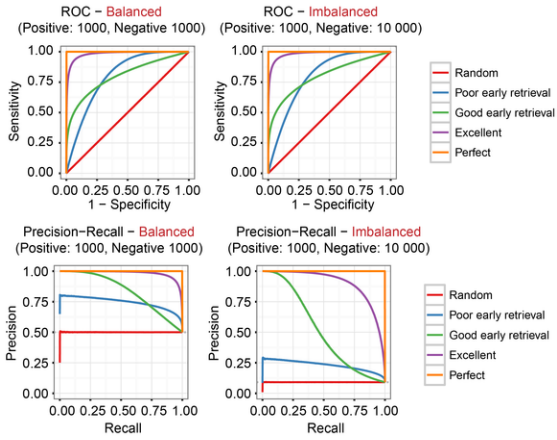

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Overfitting: how to fool the linear regression

Generalization and overfitting

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  - $y = \cos(1.5\pi x) + \mathcal{N}(0, 0.01)$, $x \sim \text{Uniform}[0, 1]$
  - Features: $\{x\}$, $\{x, x^2, x^3, x^4\}$, $\{x, \ldots, x^{15}\}$
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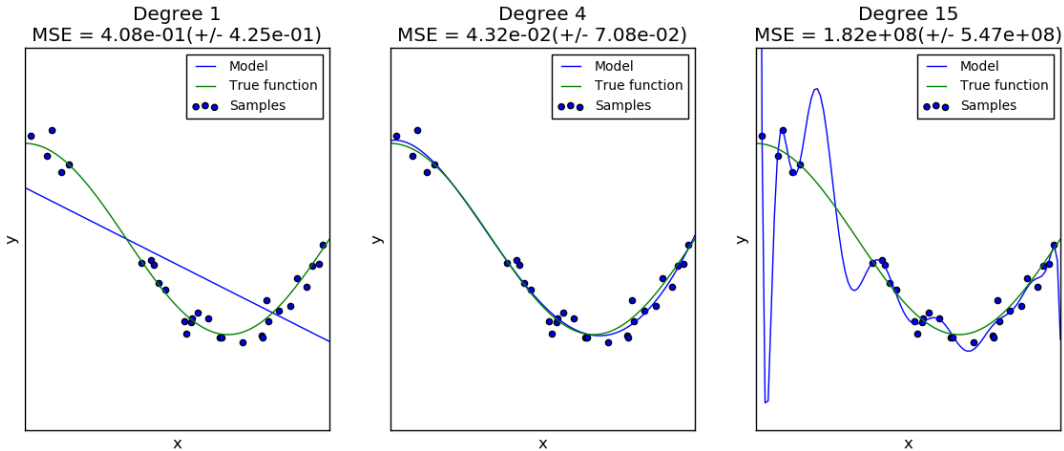
- How well do the regression models perform?

Polynomial fits of different degrees



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- The solution: rely on held-out data to assess model performance

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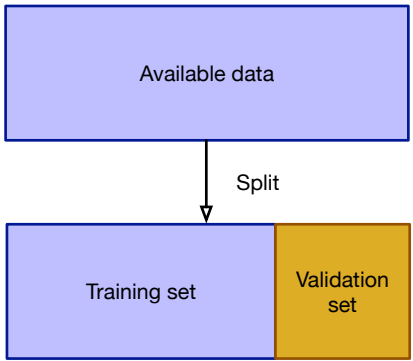
- May be imprecise: the holdout estimate of error rate will be misleading if we happen to get an "unfortunate" split



Assessing generalization ability: cross-validation

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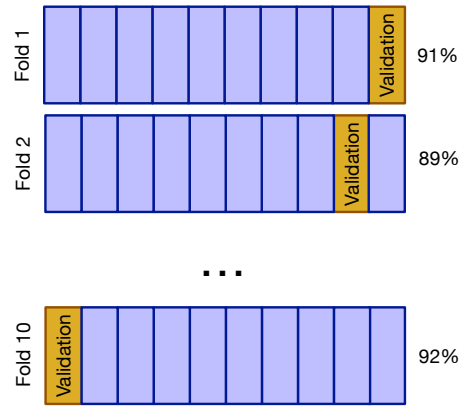
- Leave-one-out cross-validation: $X_k^\ell = \{(\mathbf{x}_k, y_k)\}$ (yes, train ℓ models!)



Cross-validation method: drawbacks

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Many folds:

- Small bias: the estimator will be very accurate
- Large variance: due to small split sizes
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- Large variance: due to small split sizes
- Costly: many experiments, large computational time

Few folds:

- Cheap, computationally effective: few experiments
- Small variance: average over many samples
- Large bias: estimated error rate conservative or smaller than the true error rate

Regularization

Ad-hoc regularization: motivation

› Consider the multivariate linear regression problem with $\boldsymbol{X} \in \mathbb{R}^{d \times d}$

$$\|\boldsymbol{y} - \boldsymbol{X}\mathbf{w}\|^2 \to \min_{\mathbf{w} \in \mathbb{R}^d}$$

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(meaning we're in eigenbasis of $\boldsymbol{X}$) then

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&= \Big(\text{diag}(\lambda_1, \ldots, \lambda_d)\text{diag}(\lambda_1, \ldots, \lambda_d)\Big)^{-1}\text{diag}(\lambda_1, \ldots, \lambda_d) = \\
&= \text{diag}\left(\frac{1}{\lambda_1}, \ldots, \frac{1}{\lambda_d}\right), \quad \text{leading to huge diagonal values in } \boldsymbol{R}
\end{aligned}$$

Ad-hoc regularization: L2

› **Regularization:** replace fit with fit + penalty as in

$$Q(\mathbf{w}) \to Q_\alpha(\mathbf{w}) = Q(\mathbf{w}) + \alpha R(\mathbf{w})$$

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- Regularized analytic solution available

$$\mathbf{w}^* = (\boldsymbol{X}^\intercal\boldsymbol{X} + \alpha\boldsymbol{I})^{-1}\boldsymbol{X}^\intercal\boldsymbol{y}$$

Why L2 regularization works

› Analytic solution: compute the regularized operator

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&= \text{diag}\left(\frac{\lambda_1}{\lambda_1^2 + \alpha}, \ldots, \frac{\lambda_d}{\lambda_d^2 + \alpha}\right),
\end{aligned}$$

smoothing diagonal values in $\boldsymbol{R}$

More regularizers!

- L2 regularized multivariate linear regression problem

$$\|\boldsymbol{y} - \boldsymbol{X}\mathbf{w}\|^2 + \alpha\|\mathbf{w}\|^2 \to \min_{\mathbf{w}\in\mathbb{R}^d}$$

- L1 regularized regression (LASSO)

$$\|\boldsymbol{y} - \boldsymbol{X}\mathbf{w}\|^2 + \alpha\|\mathbf{w}\|_1 \to \min_{\mathbf{w}\in\mathbb{R}^d}$$

- L1/L2 regularized regression (Elastic Net)

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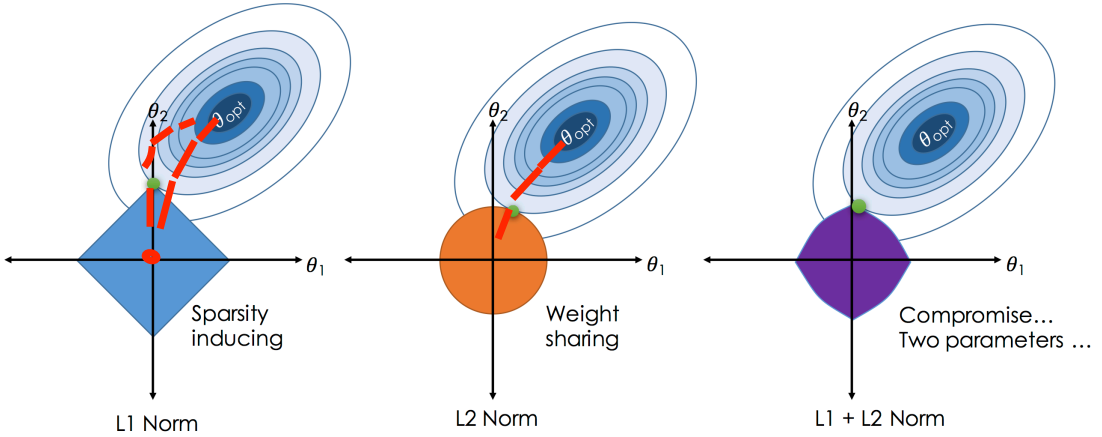
› Convex $Q(\mathbf{w})$: unconstrained optimization $Q(\mathbf{w}) + \alpha\|\mathbf{w}\|_1$ is equivalent to constrained problem $Q(\mathbf{w})$ s.t. $\|\mathbf{w}\|_1 \leqslant C$

Geometric interpretation of regularizers



Picture credit: http://www.ds100.org/sp17/assets/notebooks/linear_regression/Regularization.html

Another interpretation of regularizers

Figure: Large parameter space

Figure: Regularized models

Conclusion

- Linear models work both for regression and classification
- Main optimization methods: numerical and stochastic optimization
- Figures of merits - is not a science is an art
- Beware of overfitting! understand your data and tools
- Cross-validation is the best technique to assess your model
- Regularization is your best friend to fight overfitting