Intro into Machine Learning

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

Fifth Machine Learning in High Energy Physics Summer School,
MLHEP 2019, August 1—10

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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
- A Bayesian perspective on regularization

“Physics-based” vs. machine-learned models

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

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  - A sample from the dependency of sufficiently large size is available

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“Physics-based” vs. machine-learned models

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$$Q(h, X^\ell) = \frac{1}{\ell} \sum_{i=1}^{\ell} (f(\mathbf{x}_i) - h(\mathbf{x}_i))^2$$

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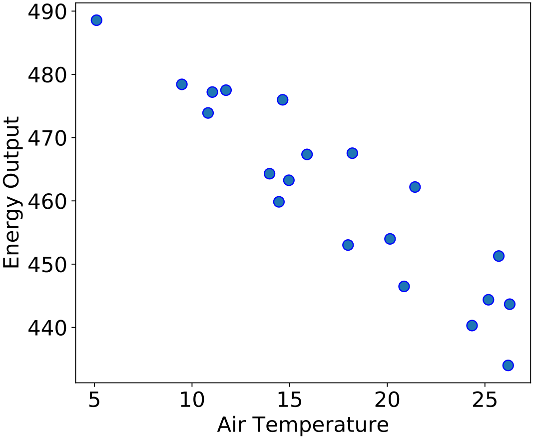
- Learning: the search for the optimal hypothesis $h \in \mathbb{H}$ w. r. t. the fixed loss function

Function approximation: energy usage



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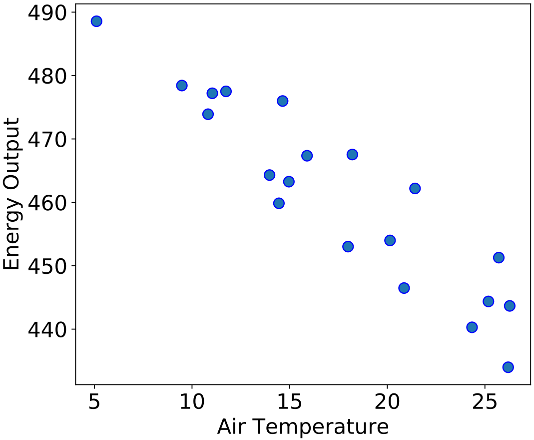

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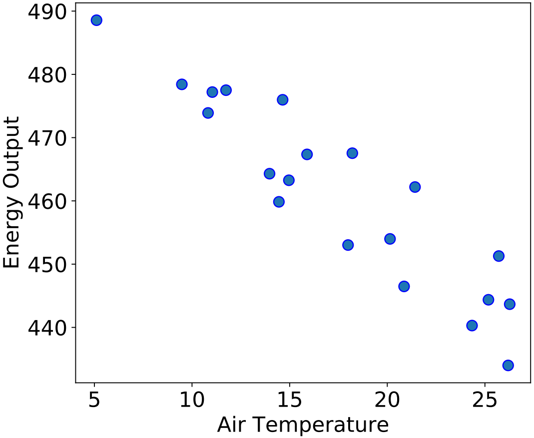

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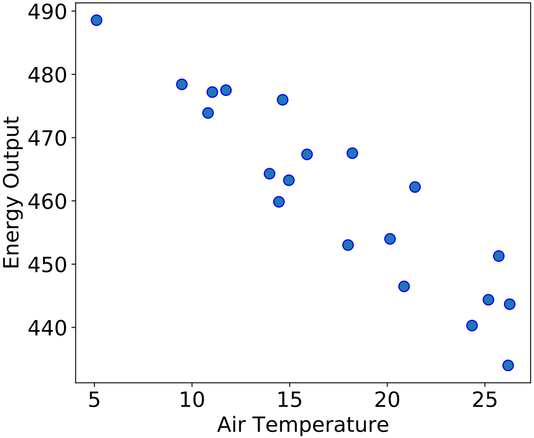

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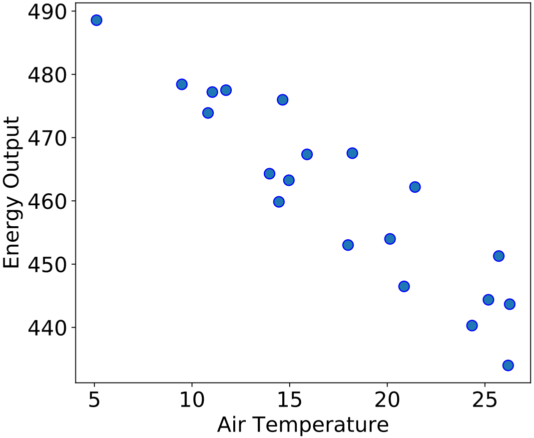

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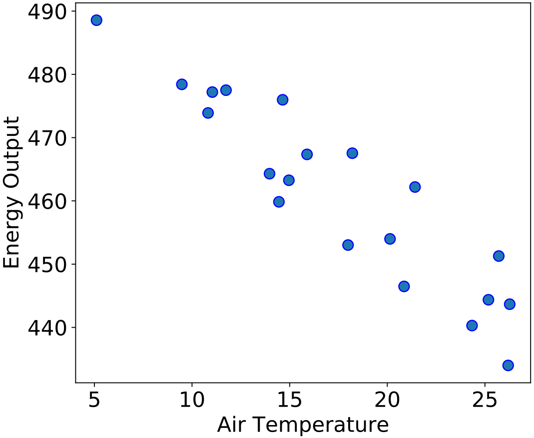

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Linear models for regression

Univariate linear regression

- A single feature (regressor) x:
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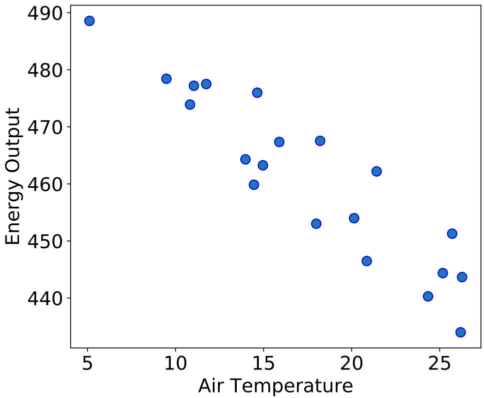

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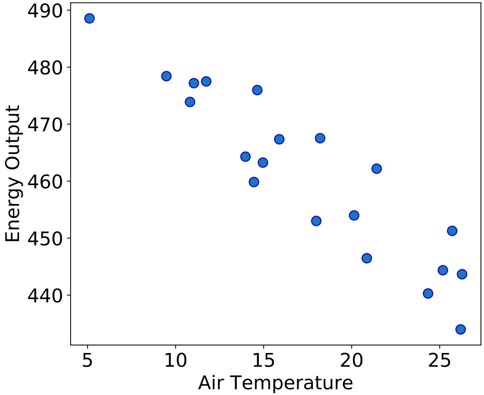

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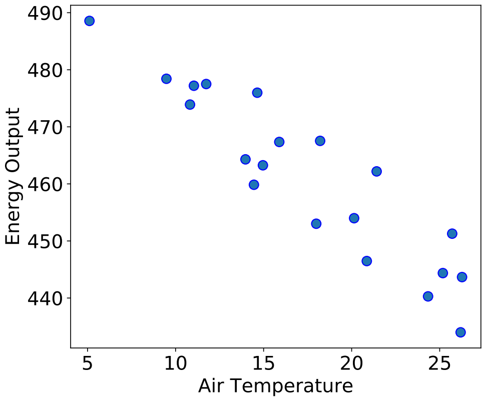

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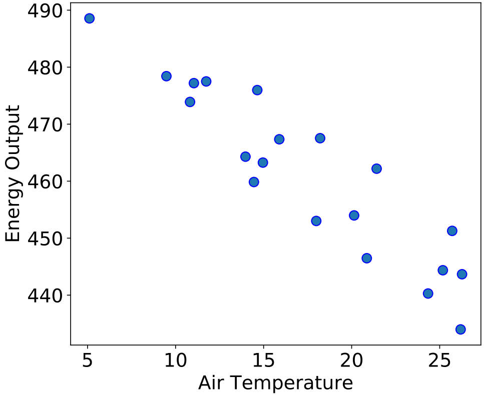

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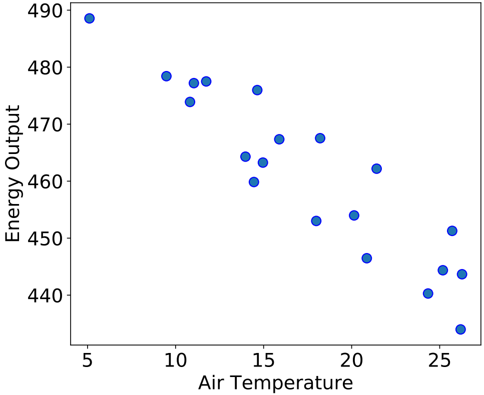

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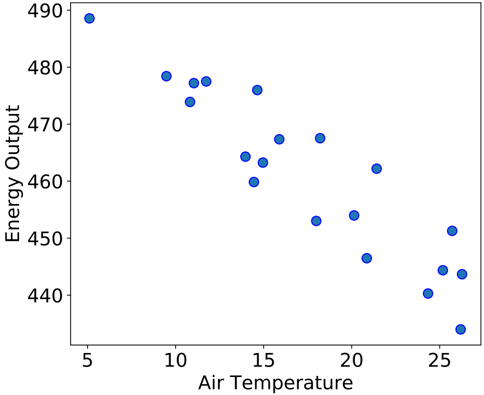
- The goal: given X^ℓ, find $\mathbf{w} = (w_1, w_0)$



Univariate linear regression

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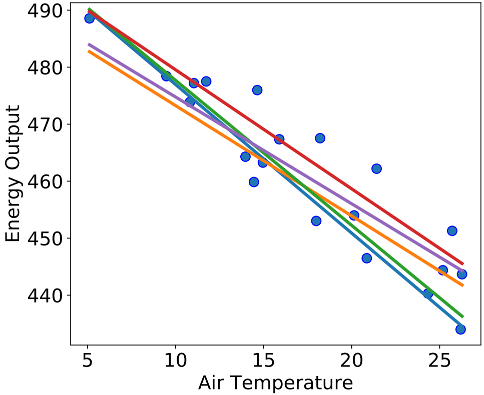

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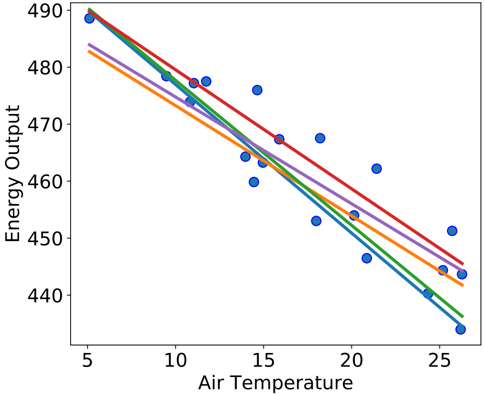

Univariate linear regression

- Which fit to choose?
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- Mean square (L2) loss (MSE):

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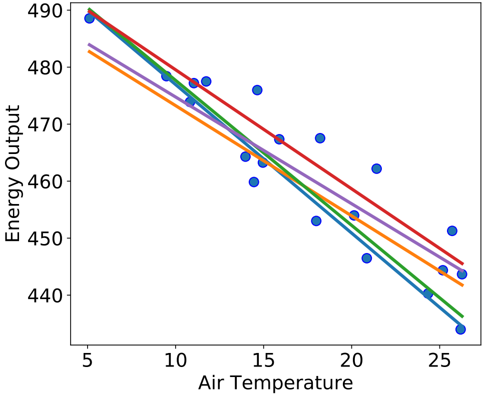

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- Coefficient of determination: $R^2(h, X^\ell) = 1 - \frac{\sum_{i=1}^{\ell}(y_i - h(x_i))^2}{\sum_{i=1}^{\ell}(y_i - \mu_y)^2}$

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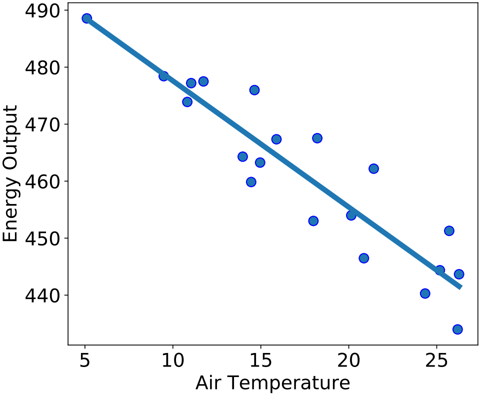
- Mean absolute error: $\mathrm{MAE}(h, X^\ell) = \frac{1}{\ell}\sum\limits_{i=1}^{\ell}|y_i - h(x_i)|$

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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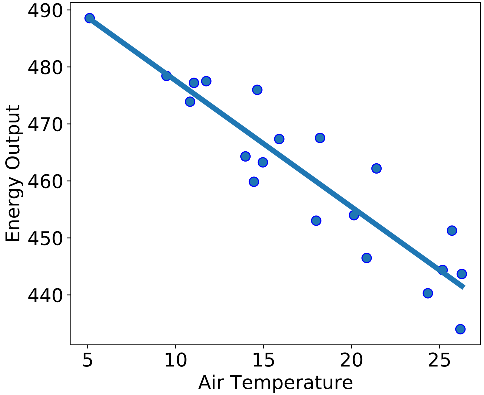
to which an analytical solution is available

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

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

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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- 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 $\mathbb{R}^d$

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

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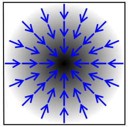
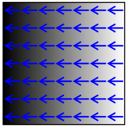
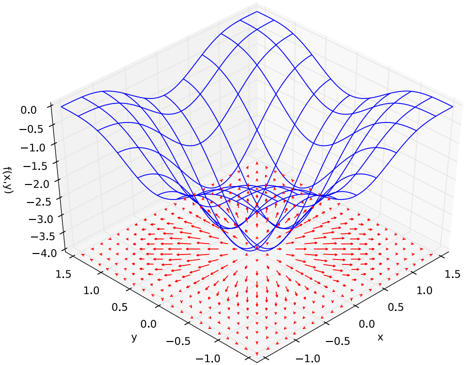
- In general, solved using the numerical methods such as the gradient descent
- Gradients: directions in $\mathbb{R}^d$ pointing towards steepest function increase

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







The gradient descent algorithm

- The gradient descent procedure iterates from $\mathbf{x}^{(0)}$ as
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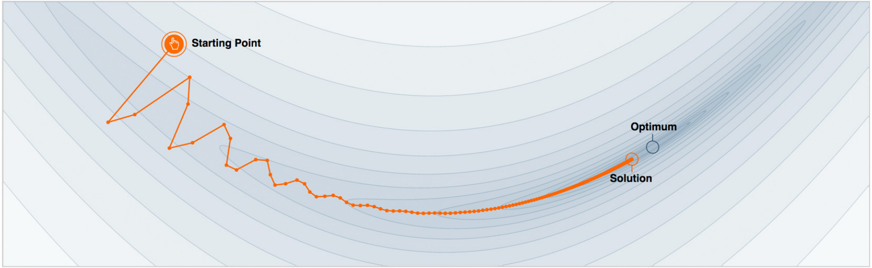
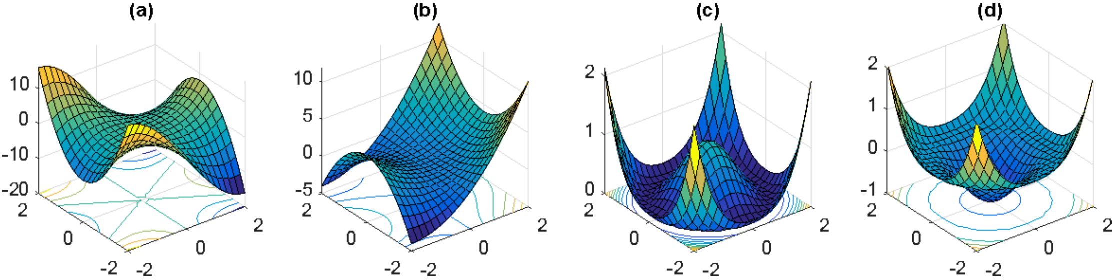
- For smooth convex functions with a single minimum $\mathbf{x}^*$, k steps of gradient descent achieve accuracy $f(\mathbf{x}^{(k)}) - f(\mathbf{x}^*) = \mathcal{O}(1/k)$



The gradient descent with non-convex targets



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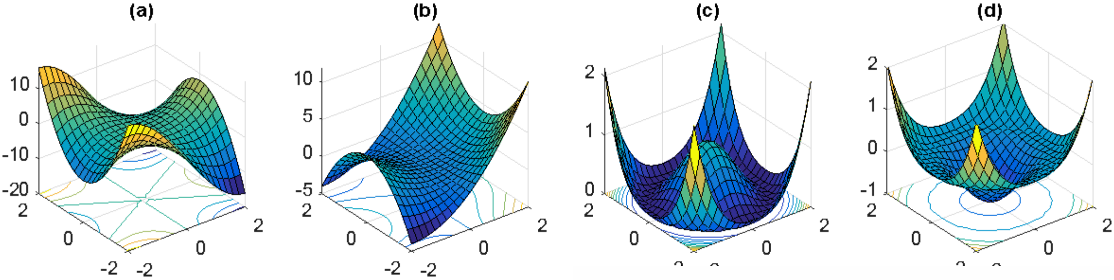
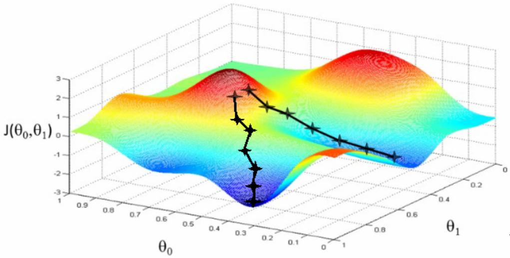


- Trajectories of gradient descent over non-convex functions may (and will) not always end up in a single optimum



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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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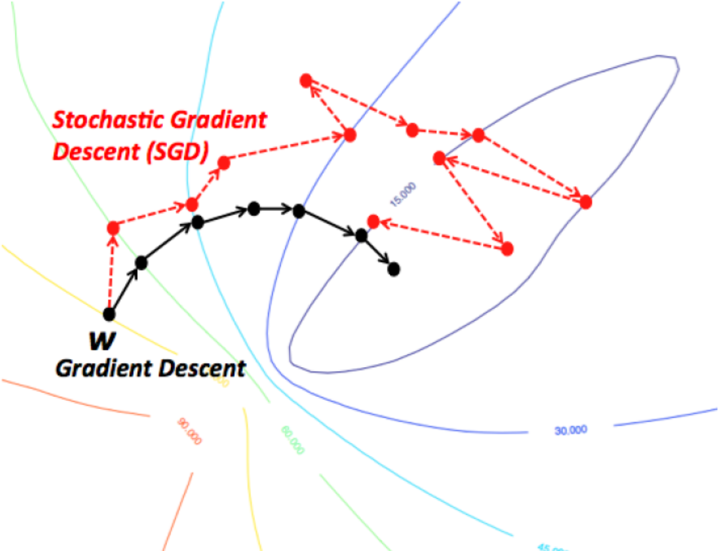
- Batching, variance reduction, momentum hacks available to improve the convergence rate to $\mathcal{O}(1/k)$

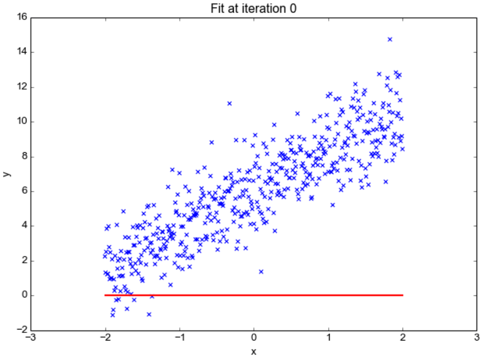
Gradient descent VS stochastic gradient descent



An example: SGD for multivariate linear regression

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

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

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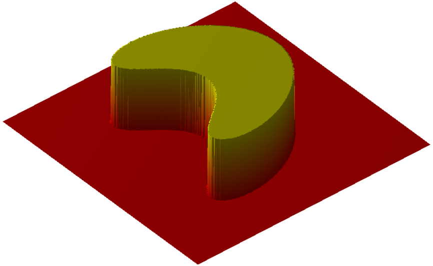

There exist sets A^+, A^- such that $A^+ \equiv \{i : \mathbf{x}_i \in D : y_i = +1\}$ and $A^- \equiv \{i : \mathbf{x}_i \in D : y_i = -1\}$ with indicator functions $\chi_{A^+}(\cdot), \chi_{A^-}(\cdot)$ (displayed on the left)

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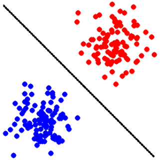
- The error of the classifier h is the probability (over D) that it will fail

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

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



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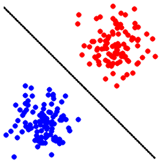

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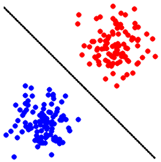

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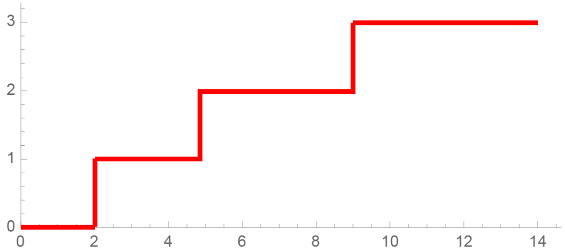

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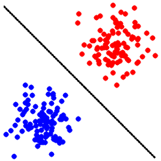

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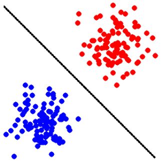

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- $Q(h, X^\ell)$ can be written using $Q(h, X^\ell) = \frac{1}{\ell} \sum_{i=1}^{\ell} L(M_i)$

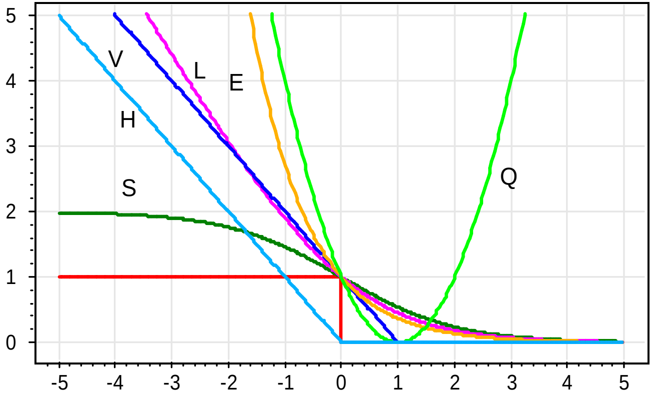
  where $L(M_i) = [M_i < 0] \equiv [y_i \mathbf{w}^\intercal \mathbf{x}_i < 0]$
- Upper-bounding $L(M)$ yields upper bounds for $Q(h, X^\ell)$

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

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

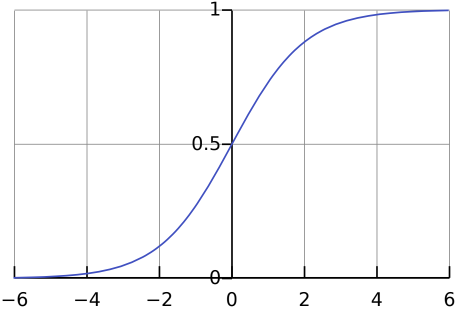
  where $\sigma(x) \in [0, 1]$

- Typical choice: the logistic function

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

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

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



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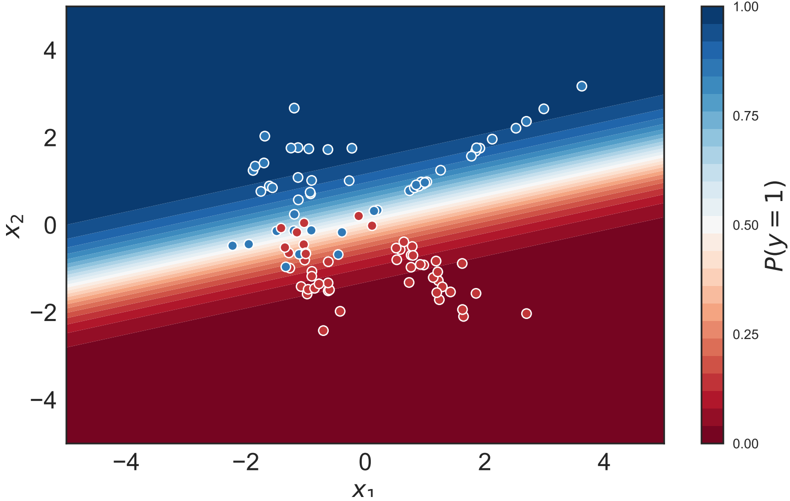

Figures of merits

Classification quality evaluation: accuracy

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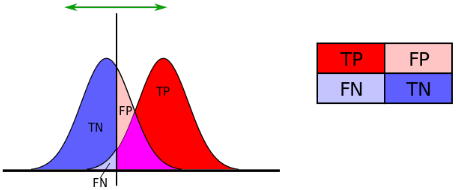
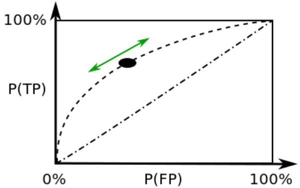
- Area under curve (ROC-AUC) reflects classification quality





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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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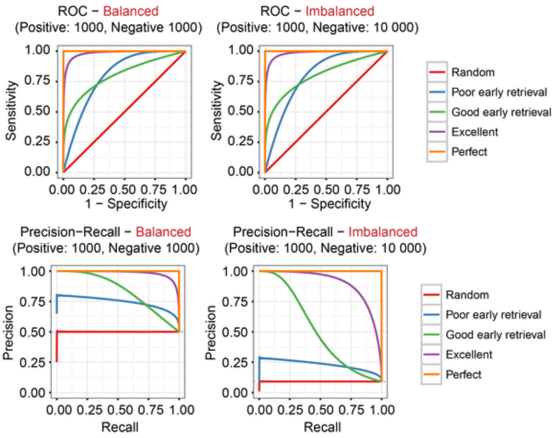

Source: classeval.wordpress.com

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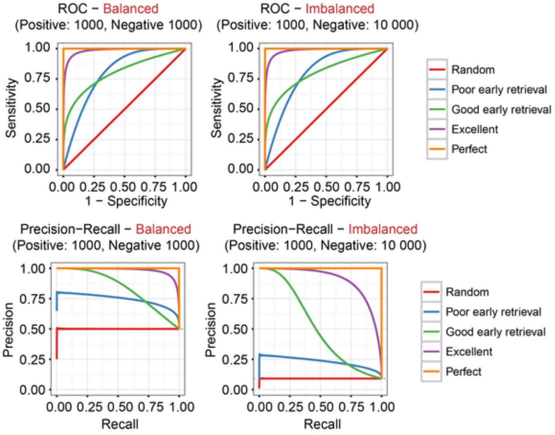

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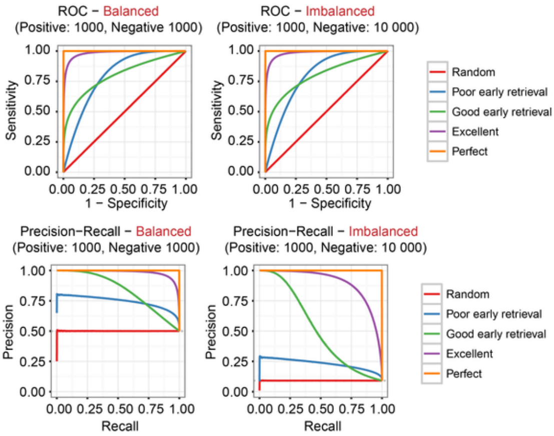

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Overfitting: how to fool the linear regression

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- Consider an example:
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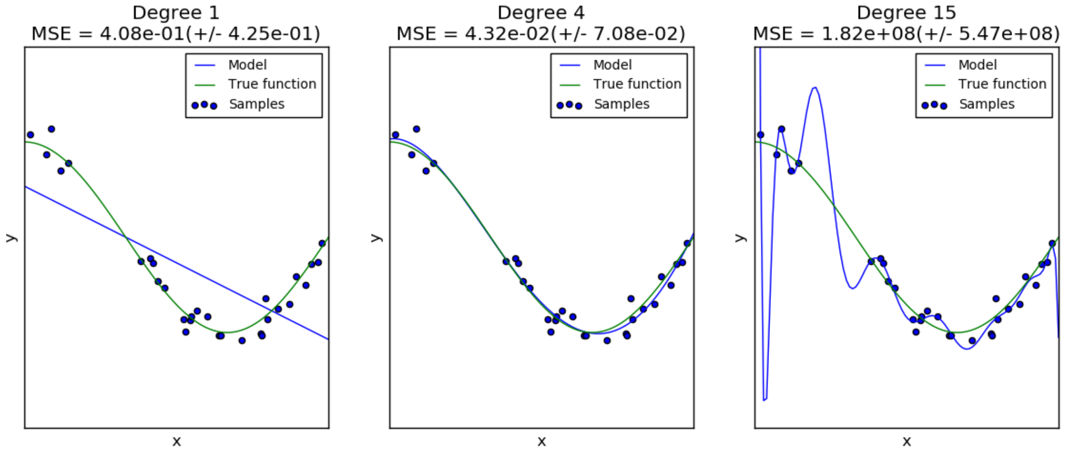
- How well do the regression models perform?

Polynomial fits of different degrees



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

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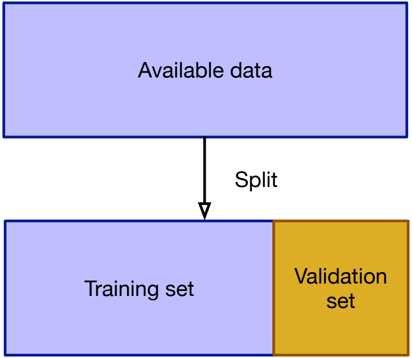

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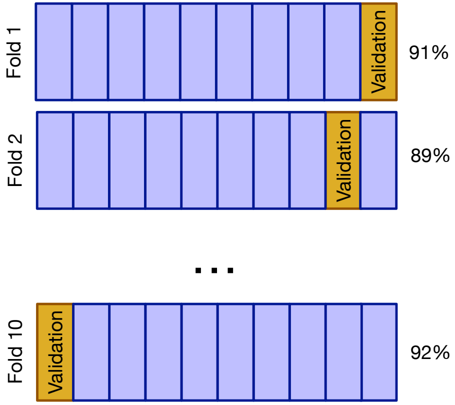
- Leave-one-out cross-validation: $X_k^\ell = \{(\mathbf{x}_k, y_k)\}$ (yes, train ℓ models!)



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- Small bias: the estimator will be very accurate
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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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- If $\boldsymbol{X} = \text{diag}(\lambda_1, \ldots, \lambda_d)$ with $\lambda_1 > \lambda_2 > \ldots > \lambda_d \to 0$ (meaning we're in eigenbasis of $\boldsymbol{X}$) then
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- **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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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)

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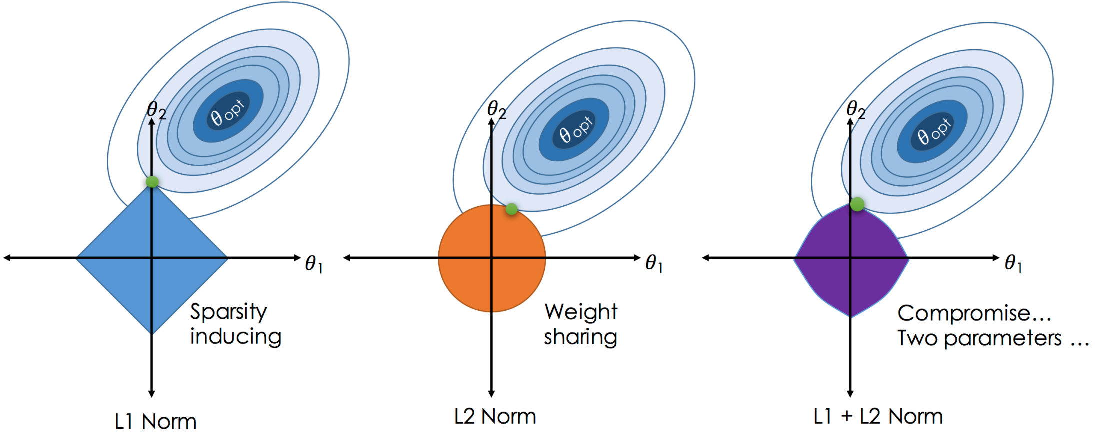
- Convex $Q(\mathbf{w})$: unconstrained optimization $Q(\mathbf{w}) + \alpha\|\mathbf{w}\|_1$ is equivalent to constrained problem $Q(\mathbf{w})$ s.t. $\|\mathbf{w}\|_1 \leqslant C$

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

A Bayesian perspective on regularization

Principled definition of regularizers?

- **L2 regularized** linear regression

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- Recall: we wanted $\mathbf{w}$ to take **small values** $\to$ α controls how small they must be
- In (Bayesian) statistics, **priors** are used to characterize variables with known (or assumed) distributions of values $\to$ use priors on weights $\mathbf{w}$!

The prior and the posterior distributions

- x is a mathematical entity

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Questions:

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- Most mathematical objects can have priors
- Sources: past experiments, expert assessment, ...

A typical scenario in Bayesian data analysis would be:

$$\boxed{\text{design a prior} \rightarrow \text{collect evidence (data)} \rightarrow \text{compute a posterior}}$$

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- Example: Gaussian $\mathbf{w} \sim \mathcal{N}(0, \sigma^2 \boldsymbol{I})$

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- Linear model for regression:

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- Likelihood for $\boldsymbol{\varepsilon}$:

$$L = \prod_i P_\varepsilon(\varepsilon_i) \implies \log L = -\sum_i \log P_\varepsilon(\varepsilon_i) = -\sum_i \log P_\varepsilon(y_i - f(x_i))$$

Prior knowledge for linear regression

› MLE for $\mathbf{w}$...

$$L = -\sum_i \log P_\varepsilon(y_i - f(x_i)) =$$

$$\sum_i \left[Z(\sigma_\varepsilon^2) - \frac{(y_i - f(x_i))^2}{2\sigma_\varepsilon^2} \right] \sim$$

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› ...is **the same as the solution for the least squares problem** (with Gaussian errors)

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- Weights prior: $\mathbf{w} \sim \mathcal{N}(0, \Sigma_w)$;
- Computing posterior we get:

$$
\begin{aligned}
P(\mathbf{w} \mid \boldsymbol{y}, \boldsymbol{X}) &\propto P(\boldsymbol{y} \mid \mathbf{w}, \boldsymbol{X}) P(\mathbf{w}) \\
&\propto \exp\left[-\frac{1}{2\sigma_\varepsilon^2}(\boldsymbol{y} - \boldsymbol{X}\mathbf{w})^T(\boldsymbol{y} - \boldsymbol{X}\mathbf{w})\right] \cdot \exp\left[-\frac{1}{2}\mathbf{w}^T \Sigma_w^{-1} \mathbf{w}\right] = \\
&\propto \exp\left[-\frac{1}{2}(\mathbf{w} - \mathbf{w}^*)^T \boldsymbol{A}_w (\mathbf{w} - \mathbf{w}^*)\right]
\end{aligned}
$$

where:

- $\boldsymbol{A}_w = \frac{1}{\sigma_\varepsilon^2}\boldsymbol{X}\boldsymbol{X}^T + \Sigma_w^{-1}$;
- $\mathbf{w}^* = \frac{1}{\sigma_\varepsilon^2}\boldsymbol{A}_w^{-1}\boldsymbol{X}\boldsymbol{y}$.