Machine Learning I Lecture VII: Logistic Regression

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Plan for today

Logistic Regression

Maximum likelihood estimation of Logistic Regression

Bayesian Logistic Regression: Approximating the posterior distribution

For the linear classification model, we assumed the class-conditional distributions to be Gaussian

- We assumed $x|(t=1) \sim \mathcal{N}(\mu_+, \Sigma_+)$ and $x|(t=-1) \sim \mathcal{N}(\mu_-, \Sigma_-)$, and two class-probabilities $P(t=1)$ and $P(t=-1)$.

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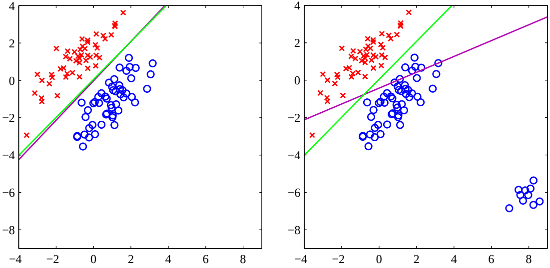
- This is called an generative model, as we have written down a full joint model over the data.
- We saw that violations of the model assumption can lead to 'bad' decision boundaries.



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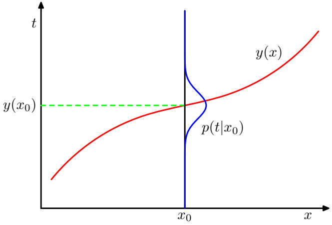
- We maximized the conditional log-likelihood $L(\omega) = \sum_n \log p(t_n|x_n, \omega)$, i.e we assumed that the x were given.
- Therefore, this approach to linear regression works for any distribution over x.
- x is typically high-dimensional, so it is difficult to make appropriate distributional assumptions for it.



We can define a discriminative model for classification by modelling the conditional class probabilities.

- From the homework-exercise, we know that $P(t = 1|z(x)) = \sigma(z(x))$ where $\sigma(z) = 1/(1 + \exp(-z))$ and $z(x) = \omega^\top x + \omega_o$.
- Notation is simpler if we use 0 and 1 as class labels, so we define $s_n = 1$ as the label for the positive class, and $s_n = 0$ als label for the negative class.
- In other words, $s|x \sim \text{Bernoulli}(\sigma(y(x))$.
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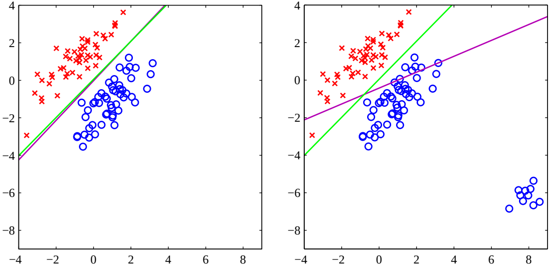
- This is an discriminative approach to classification, as we only model the labels, and not the inputs.
- Decision rule and function shape of $p(t|x)$ will be the same for the generative ('Linear Discriminant Analysis') and the discriminative model, but the parameters were obtained differently.

Maximum likelihood estimation of Logistic Regression



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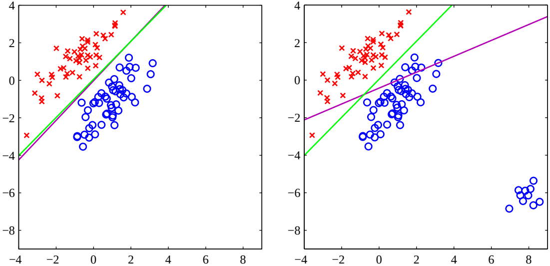

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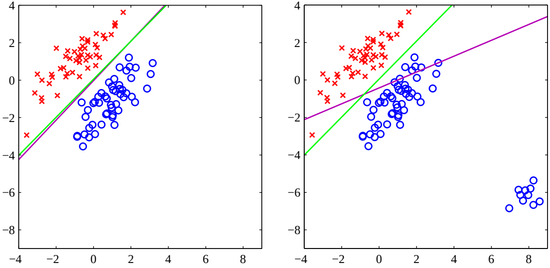

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- Need to optimize log-likelihood numerically.
- People typically minimize the negative log-likelihood $\mathcal{L}$ rather than maximize the log-likelihood...
- To numerically minimize the negative log-likelihood, we need its gradient (and maybe its hessian) [on board]

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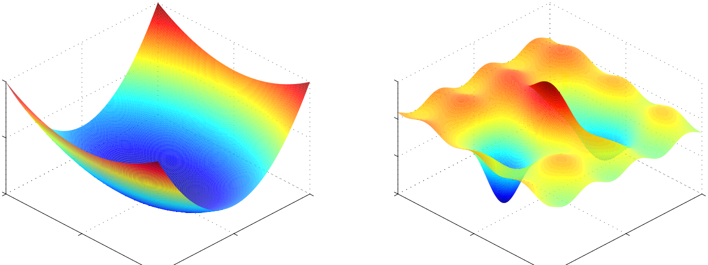

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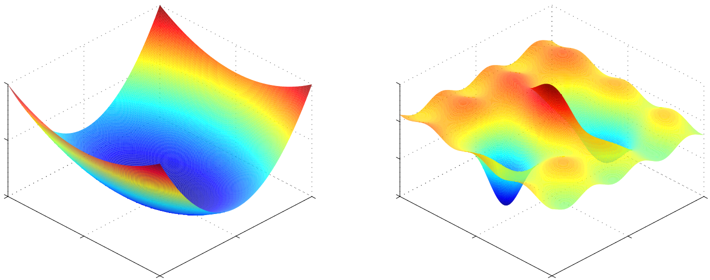

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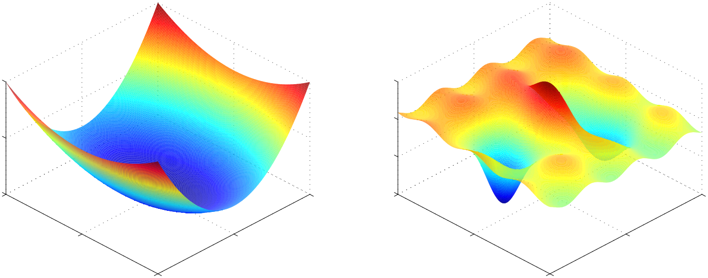

- Fact: The negative log-likelihood is *convex* – this makes life much more easier.
- There are no local minima to get stuck in, and there is good optimization techniques for convex problems.

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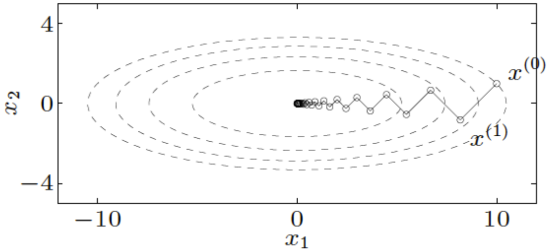
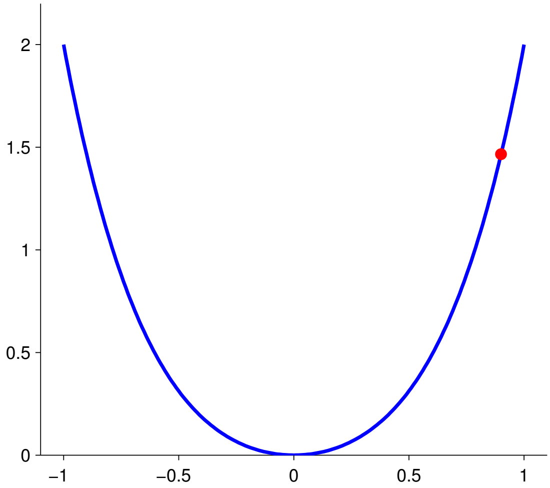
- Convergence can be very slow if cost-function has 'valleys'.



Iterative Least Squares: Approximate by parabola, minimze, iterate.



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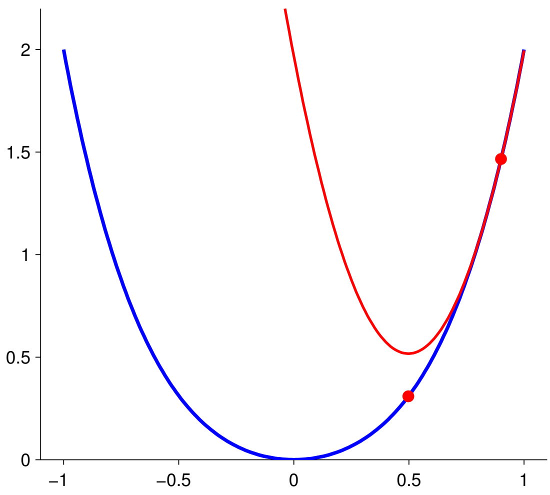

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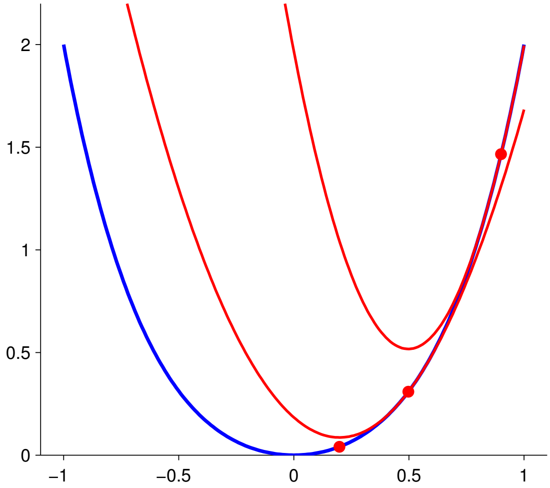

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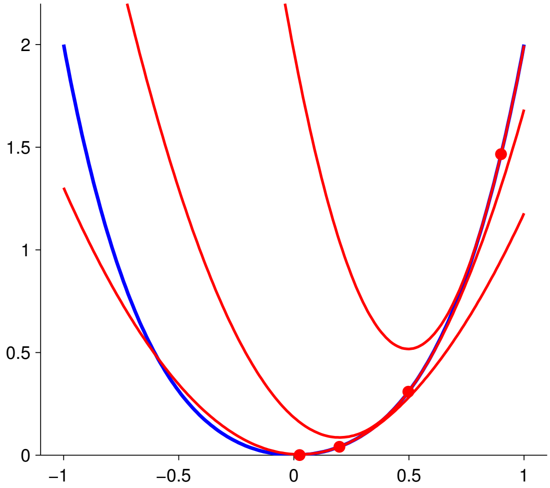

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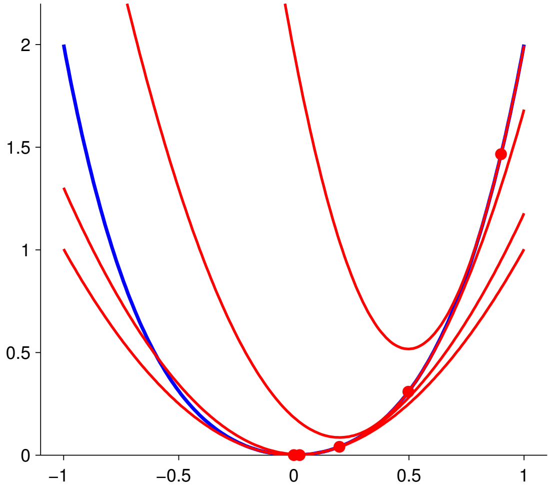

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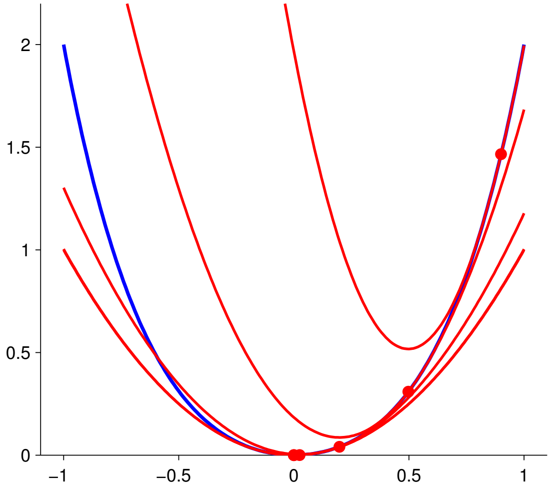

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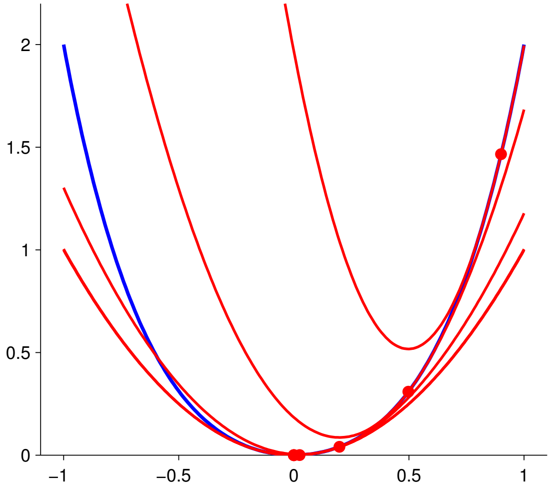

Iterative Least Squares is a more efficient method for minimizing the cost-function

- Newton-Raphson: $\omega_{new} = \omega_{old} - \alpha(\nabla\nabla\mathcal{L})^{-1}\nabla L_\omega$
- Pre-multiplying the gradient by the inverse-hessian speeds up convergence 'along valleys' (analogy with LDA)
- Motivation: For quadratic functions $F(x) = a + b^\top x + x^\top Bx$, Newton-Raphson finds the minimum in one iteration.
- In this contex, Newton-Raphson (with $\alpha = 1$) is often called iterative least squares.
- Note: Newtwn's method can be bad if problem is not convex, and can be slow if it is difficult to calculate/invert the Hessian. A large number of optimization algorithms exist which do not require the (complete) Hessian (quasi Newton/BFGS, etc..).

Visualizing the cost-function of logistic regression

[on board]

Bayesian inference for this model does not have a closed form solution

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- Different methods exist for finding 'good' μ_{post} and Σ_{post}: Expectation Propagation (EP), Laplace Approximation, Variational Inference

The Laplace-Approximation is a simple Gaussian approximation to the posterior

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- Take MAP as mean, and inverse hessian at MAP as covariance.

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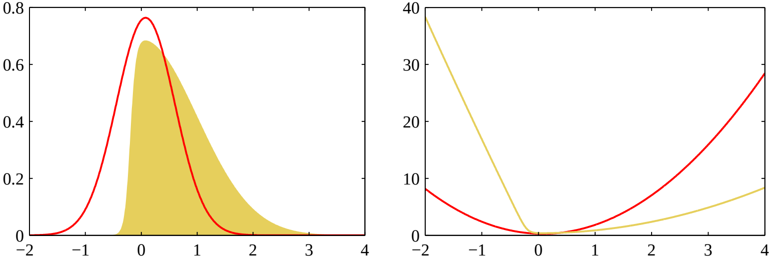
- Q: When will the Laplace approximation fail?



The posterior distribution can be used to calculate the predictive distribution and to optimze hyper-parameters

[on board]

One last bit of business: The exam

- Next Friday, 2pm *sharp*.
- You will have 90 minutes.
- You are allowed to use a pen or other writing utensils and your brain, no other tools/materials/books/notes will be allowed. All mobiles phones need to be switched off.
- Master-Students: Graded
- Everyone else: Pass/Fail. If you want a grade for whatever reason, let me know (but tit might not have any official meaning).

This is the end.

Have fun in the second half of the course!

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If you did like (some bits) from these lectures ...

... and want to do a lab-rotation on using machine-learning methods to analyse neural data and to model neural population dynamics

... write an email to jakobtuebingen.mpg.de.