Nonlinear Fits: Challenges and algorithms

Intro

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I did my PhD with Phil Anderson. He had an amazing track record of ideas that have shaped physics.

We are gathered here to explain why nature is comprehensible. As Eugene Wigner asked, why does mathematics describe the natural world? Phil Anderson asserted that there are emergent laws describing the collective behavior of complex systems — that the laws governing our economy or ecosystem are every bit as ‘fundamental’ as those of high-energy physics.

Today I want to introduce a different kind of emergence. We shall use information geometry and a kind of interpolation theory to show that complex systems with many microscopic parameters will quite generally exhibit comprehensible collective behaviors.

Gets stuck at bad fit

- Usually not lots of local minima!
  - Sloppy directions co-dimension argument
  - Robustness to external conditions
- Lost on plateaus
- Twisty rivers at bottom

If most of the 48 dimensions of parameter space are sloppy, why not develop simpler models with fewer parameters?

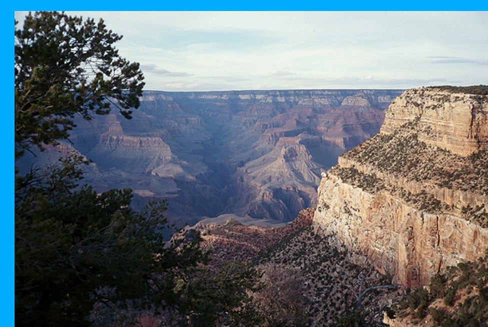
Exploring Parameter Space

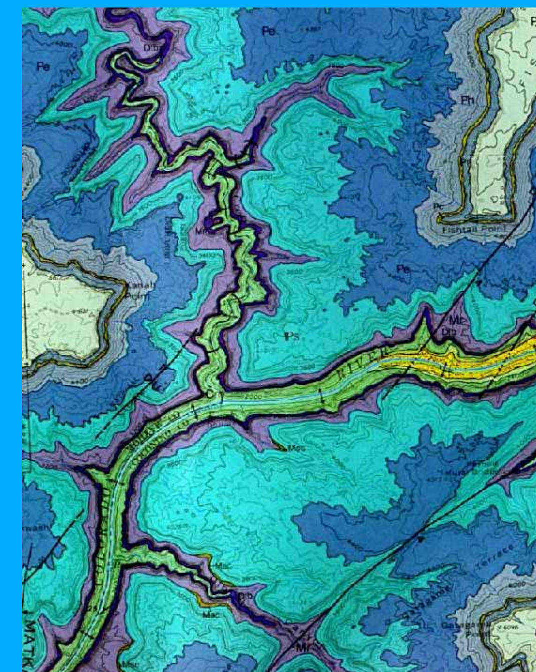
Rugged? More like Grand Canyon (Josh)

Glasses: Rugged Landscape
- Metastable Local Valleys
- Transition State Passes

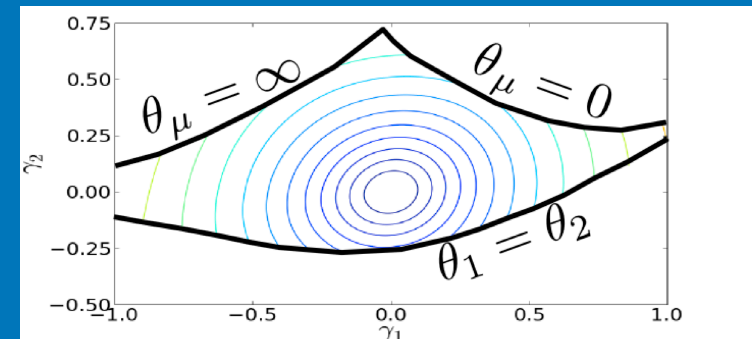
Optimization Hell: Golf Course

Sloppy Models
- Minima: 5 stiff, N-5 sloppy
- Search: Flat planes with cliffs





Finding best fit not hard in behavior space



The cost contours on the model manifold are concentric spheres near the best fit.

Cost Contours in Behavior Space

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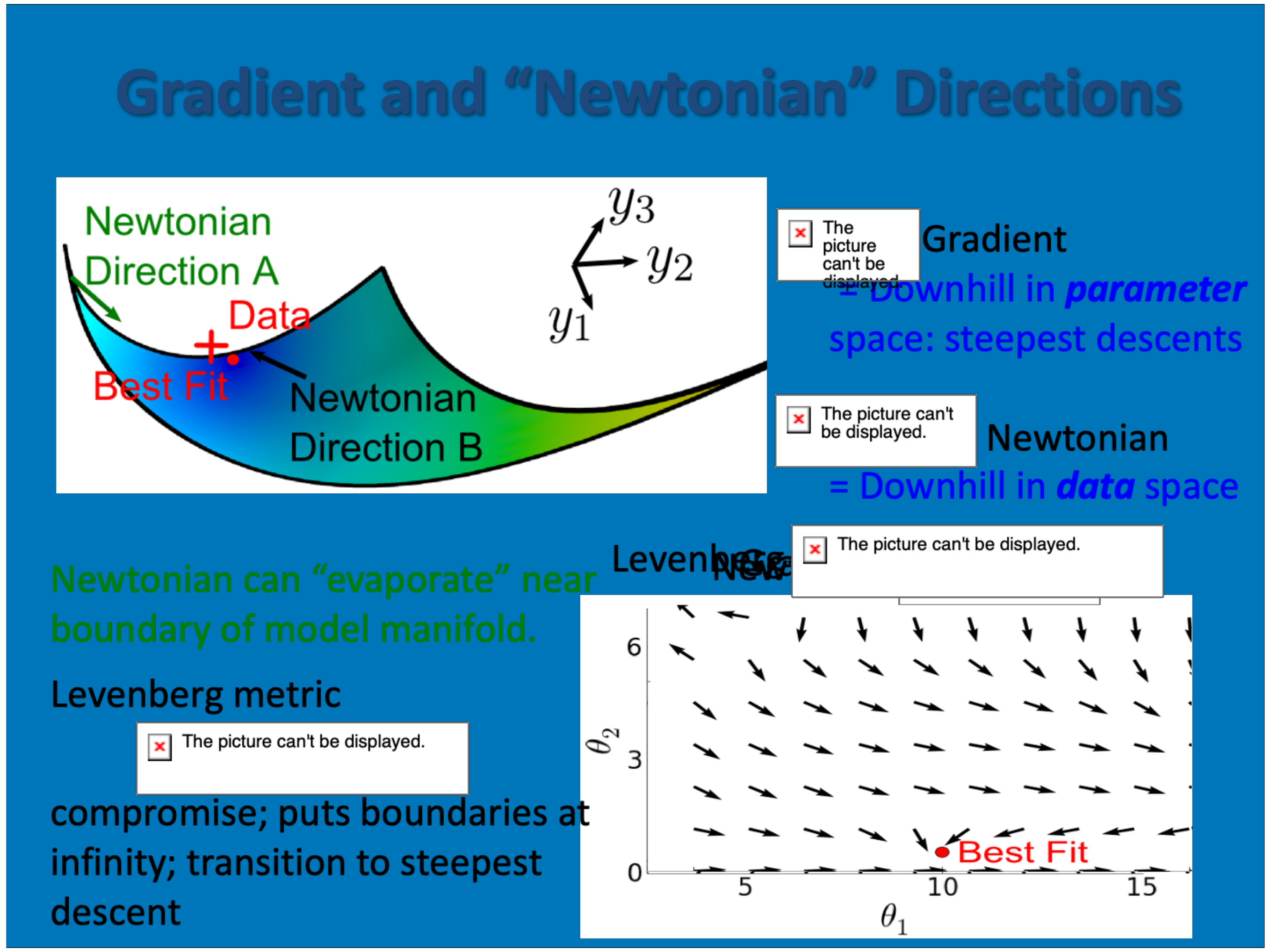

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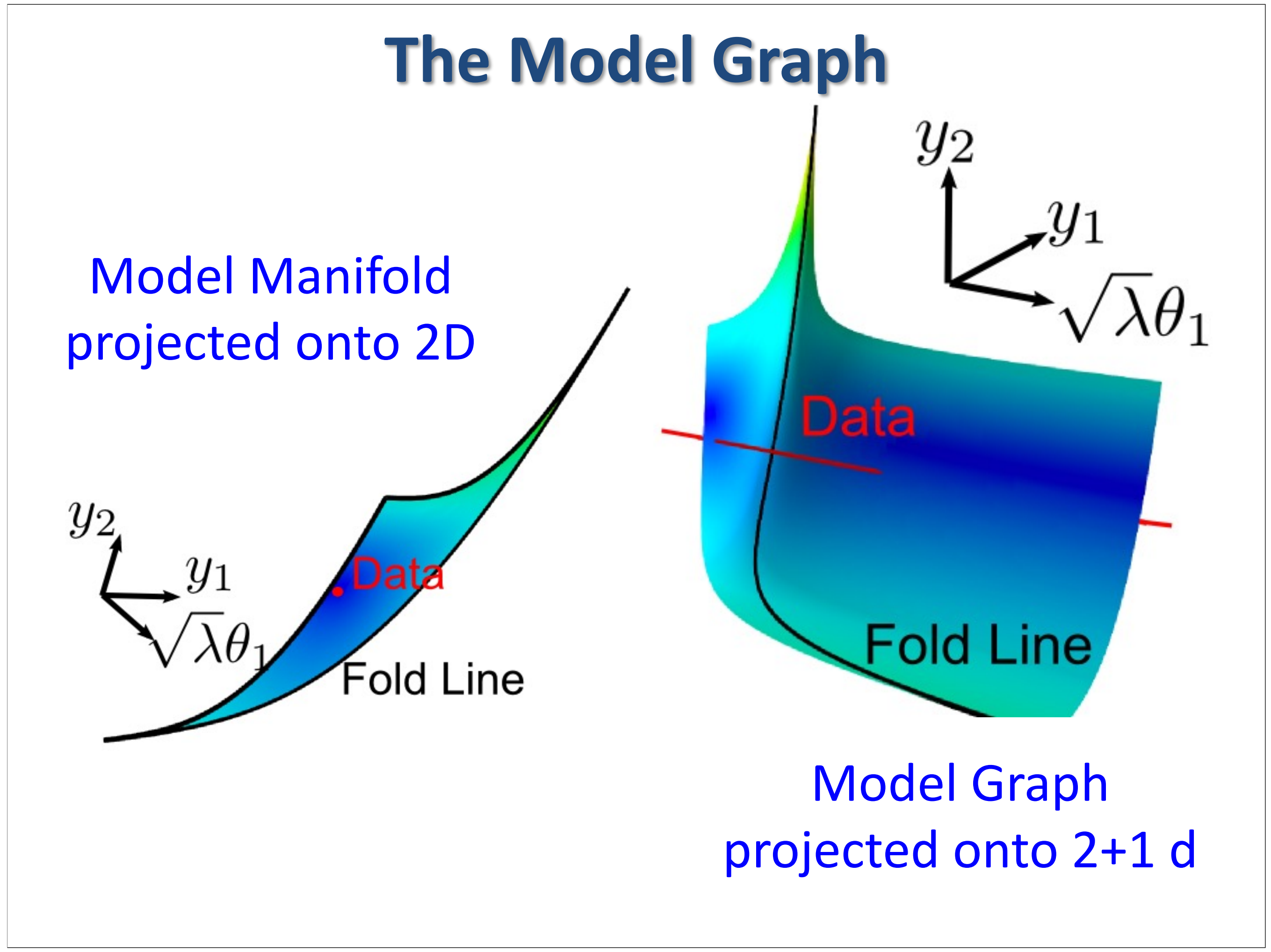

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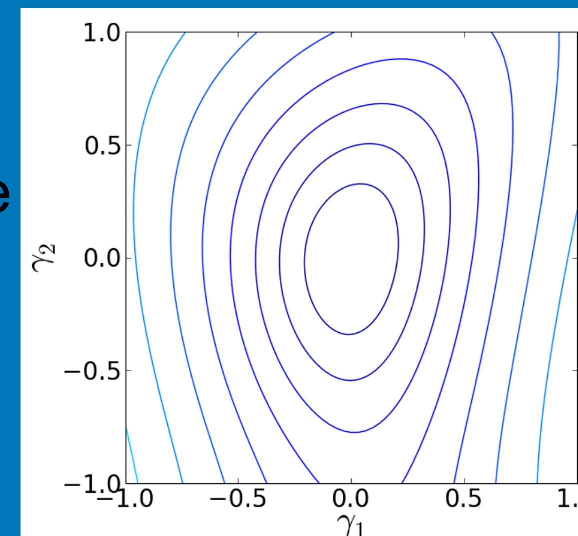
Finding best fit not hard in behavior space

The cost contours on the model graph are concentric spheres for small λ, parameter-space contours for large λ. (Here shifted to log parameters, so sloppiness and plateau not as apparent.)



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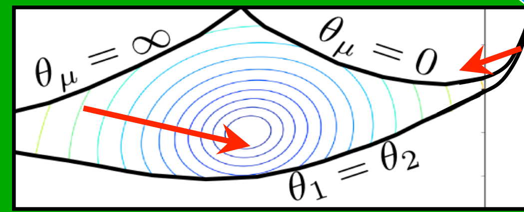
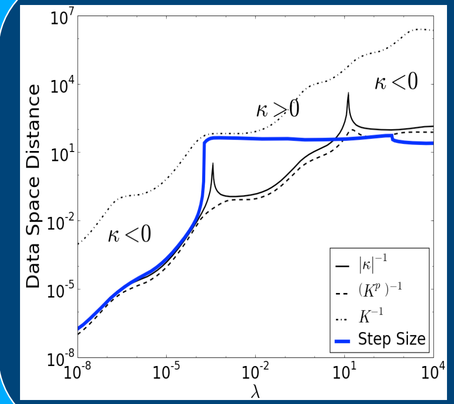
B. Finding best fits: Geodesic acceleration



Geodesic Paths nearly circles
Follow local geodesic velocity?

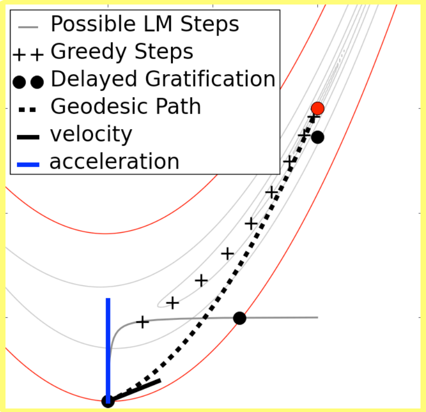
$$\delta\theta^{\mu} = -g_{\mu\nu}\nabla_{\nu}C$$

- ➔ Gauss-Newton
- ➔ Hits manifold boundary



Model Graph

add weight λ of parameter metric yields Levenberg-Marquardt: Step size now limited by curvature

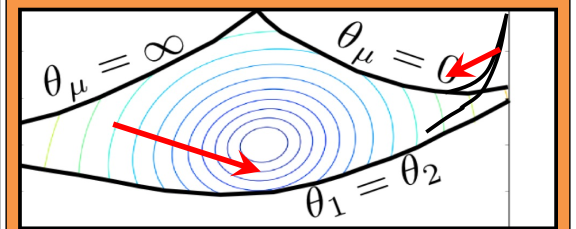


Algorithm	Success Rate	Mean njev	Mean nfev
Traditional LM + accel	65%	258	1494
Traditional LM	33%	2002	4003
Trust Region LM	12%	1517	1649
BFGS	8%	5363	5365

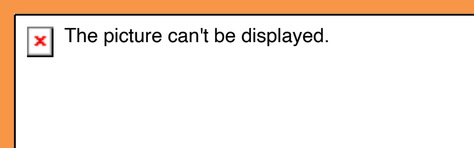
Follow parabola, ***geodesic acceleration***

Cheap to calculate; faster; more success

Finding best fits: Geodesic acceleration



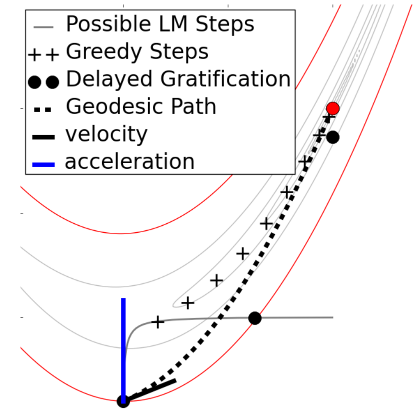
Geodesic Paths nearly circles (small λ)
Follow local geodesic downhill?



Geodesic acceleration

$a^\mu = -\Gamma^\mu_{\alpha\beta} v^\alpha v^\beta$

(quadratic approximation to geodesic equation)



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LM = Downhill on MG
Yellow sticky section
Delayed gratification
Geodesic Acceleration
(Not much faster, but doesn’t get stuck as often)

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Applications not discussed here

Dynamical systems:

  Lyapunov and structural susceptibility (Chachra, Transtrum)

Power system dynamics (Transtrum)

Optimal experimental design (Casey, Cerione; Tidor et al.)

Control theory

Nuclear physics

Protein allostery

Heart dynamics