Numerical Optimization using the Levenberg-Marquardt Algorithm

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The Basic Least-Squares Problem

$$r_m = y_m - f(t_m, \theta)$$

$$C = \sum_m r_m(\theta)^2$$

Find the values of $\theta_1,\ \theta_2,\ \theta_3,\ \ldots,\ \theta_n$ such that C is minimized.

Optimization Algorithms

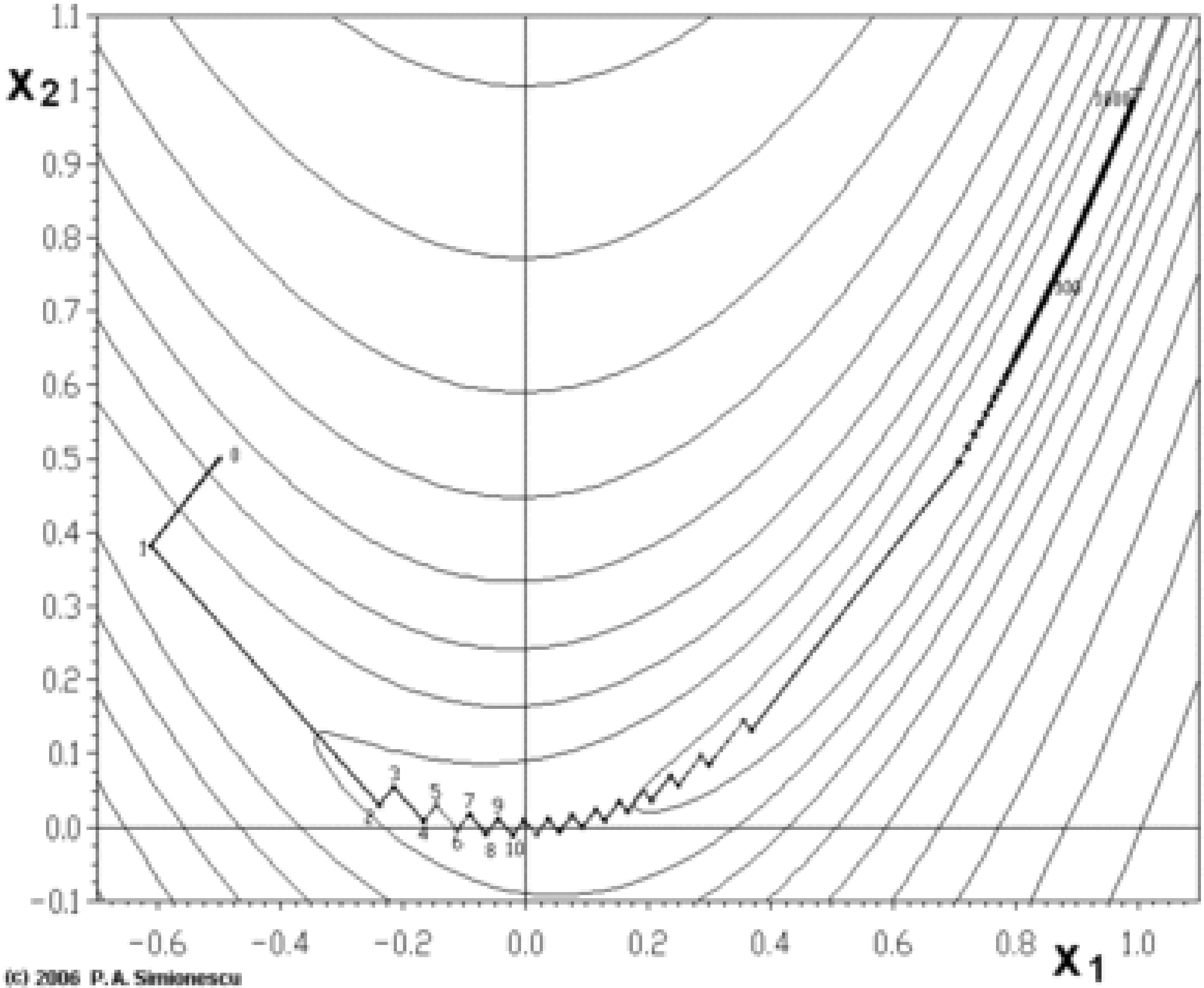
Gradient descent : Start with an initial guess x_0.

$$x_{n+1} = x_n - \gamma_n \nabla F(x_n),\ n \geq 0$$

Advantages: F(x) will decrease after every iteration.
-Decreases cost most quickly for a given change in parameter values.
Disadvantages: Algorithm tends to zigzag along the bottom of long narrow canyons. Approaches the best fit very slowly.

Gradient descent = Steepest descent = First-order gradient-based method

Source: Wikipedia



x_2
x_1
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
-0.1
-0.6
-0.4
-0.2
0.0
0.2
0.4
0.6
0.8
1.0
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Optimization Algorithms

Gauss - Newton: Start with an initial guess x_0.

Adjust x by Δ at each step, where Δ is given by solving:

$(J_f^T J_f)\Delta = J_f^T r$ for data fitting problems, $(J_r^T J_r)\Delta = J_r^T r$

for minimizing functions.

Advantages: Decreases cost most efficiently for a change in its behavior.

-Converges quickly in canyons

Disadvantages: Prone to parameter evaporation (parameters returned by the algorithm are far from reasonable values).

-Algorithm converges slowly or not at all if initial guess is far from minimum or matrix is ill-conditioned.

(JTJ) applied to approximate second-order Hessian matrix.

Gauss-Newton = Second-order curvature-based method

Source: Wikipedia

The Levenberg-Marquardt Algorithm

LM algorithm combines the advantages of gradient-descent and Gauss-Newton methods.

-LM steps are linear combination of Gradient-descent and Gauss-Newton steps based on adaptive rules

Gradient-descent dominated steps until the canyon is reached, followed by Gauss-Newton dominated steps.

The Levenberg-Marquardt Algorithm

Start with an initial guess x_0. x is adjusted by δ only for downhill steps.

$$(J^T J + \lambda I)\delta = J^T r$$

J = jacobian matrix of derivatives of the residuals with respect to the parameters
λ = damping parameter (adaptive balance between the 2 steps)
r = residual vector

Description (pseudocode) of the LM algorithm – from Transtrum, Machta, Sethna, 2011

1. Initialize values for the parameters, x, the Levenberg-Marquardt parameter λ, as well as λ_{up} and λ_{down} to be used to adjust the damping term. Evaluate the residuals r and the Jacobian J at the initial parameter guess.
2. Calculate the metric, $g = J^T J + \lambda I$, and the cost gradient, $\nabla C = J^T r$, $C = \frac{1}{2} r^2$.
3. Evaluate the new residuals r_{new} at the point given by $x_{new} = x - g^{-1} \nabla C$, and calculate the cost at the new point, $C_{new} = \frac{1}{2} r_{new}^2$.
4. If $C_{new} < C$, accept the step, $x = x_{new}$, and set $r = r_{new}$ and $\lambda = \lambda / \lambda_{down}$. Otherwise, reject the step, keep the old parameter guess x and the old residuals r, and adjust $\lambda = \lambda \times \lambda_{up}$.
5. Check for convergence. If the method has converged, return x as the best-fit parameters. If the method has not yet converged but the step was accepted, evaluate the Jacobian J at the new parameter values. Go to step 2.

LevMar Convergence Criteria as implemented in MADS

Algorithm stops when:

1. Objective function value is below a cutoff value (if specified) OR
2. $J^T r$ is small (max element <= eps) OR
3. Relative change in p is small ($\le eps^2||p||$) OR
4. Almost singular solution OR
5. Model predictions are within a certain range of the true minimizer (if provided) OR
6. Algorithm returns invalid (NaN or inf) values OR
7. Maximum number of iterations is reached.

Choosing the Damping Parameter (λ)

- Choice of λ is very important for success rate and efficiency of the LM algorithm.
- Increasing λ decreases step size, and vice versa. So if a step is unacceptable, λ should be increased until a smaller, acceptable step is found. If a step is accepted, we want to increase step size by decreasing λ, in order to proceed more quickly in the correct descent direction, speeding up convergence rate.

Source: Transtrum PhD dissertation, 2011

Schemes for Updating λ

- Direct method – increase λ by a fixed factor for uphill steps, decrease λ by the same fixed factor for downhill steps.
- Direct method/Delayed gratification – increase λ by a small fixed factor for uphill steps, decrease λ by a larger fixed factor for downhill steps.
- Indirect method – choose an initial step size Δ, then find a λ such that $|\delta\theta| \leq \Delta$

Source: Transtrum dissertation, Transtrum, Machta, Sethna, 2011

Motivation for Delayed Gratification Method

- Direct method with equal up and down adjustments tends to move downhill too quickly, greatly reducing steps that will be allowed at successive iterations, which slows convergence rate (although it appears to have no effect on success rate).
- By using delayed gratification, we choose the smallest λ that does not produce an uphill step, which slows initial downhill progression but speeds up convergence rate near the solution.

Source: Transtrum, Machta, Sethna, 2011

Test Function	Method	Success Rate	Av. Jacobian Evals.
Rosenbrock	Direct	0.987	17.9
	Delayed Gratification	0.965	13.4
	Indirect	0.946	32.6
Powell's Quadratic	Direct	0.783	11.8
	Delayed Gratification	0.812	10.9
	Indirect	0.643	62.1
Exponential Data Fitting I	Direct	0.017	61.7
	Delayed Gratification	0.161	38.5
	Indirect	0.054	42.3
Exponential Data Fitting II	Direct	0.009	138
	Delayed Gratification	0.008	73.2

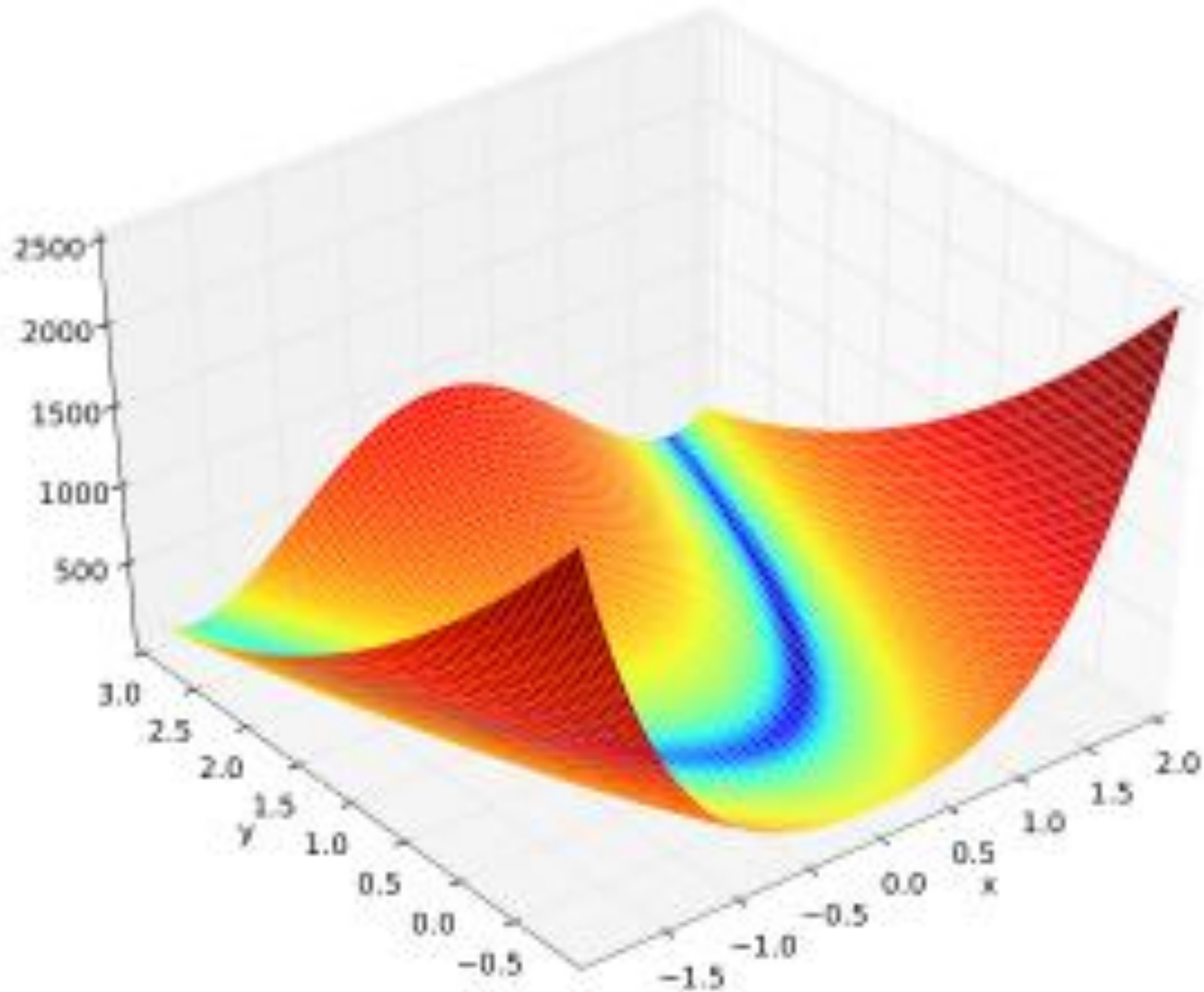
The Rosenbrock Function

$$f(x,y) = (1-x)^2 + A(y-x^2)^2$$

A controls the narrowness of the canyon

Ideal for testing optimization algorithms because of the difficulty of convergence. Finding the valley that contains the global minimum (1, 1) is trivial, but moving along the valley to the minimum is very difficult.
No local minima, though higher dimensional forms contain several at unknown locations, making it difficult to test them for success rate.

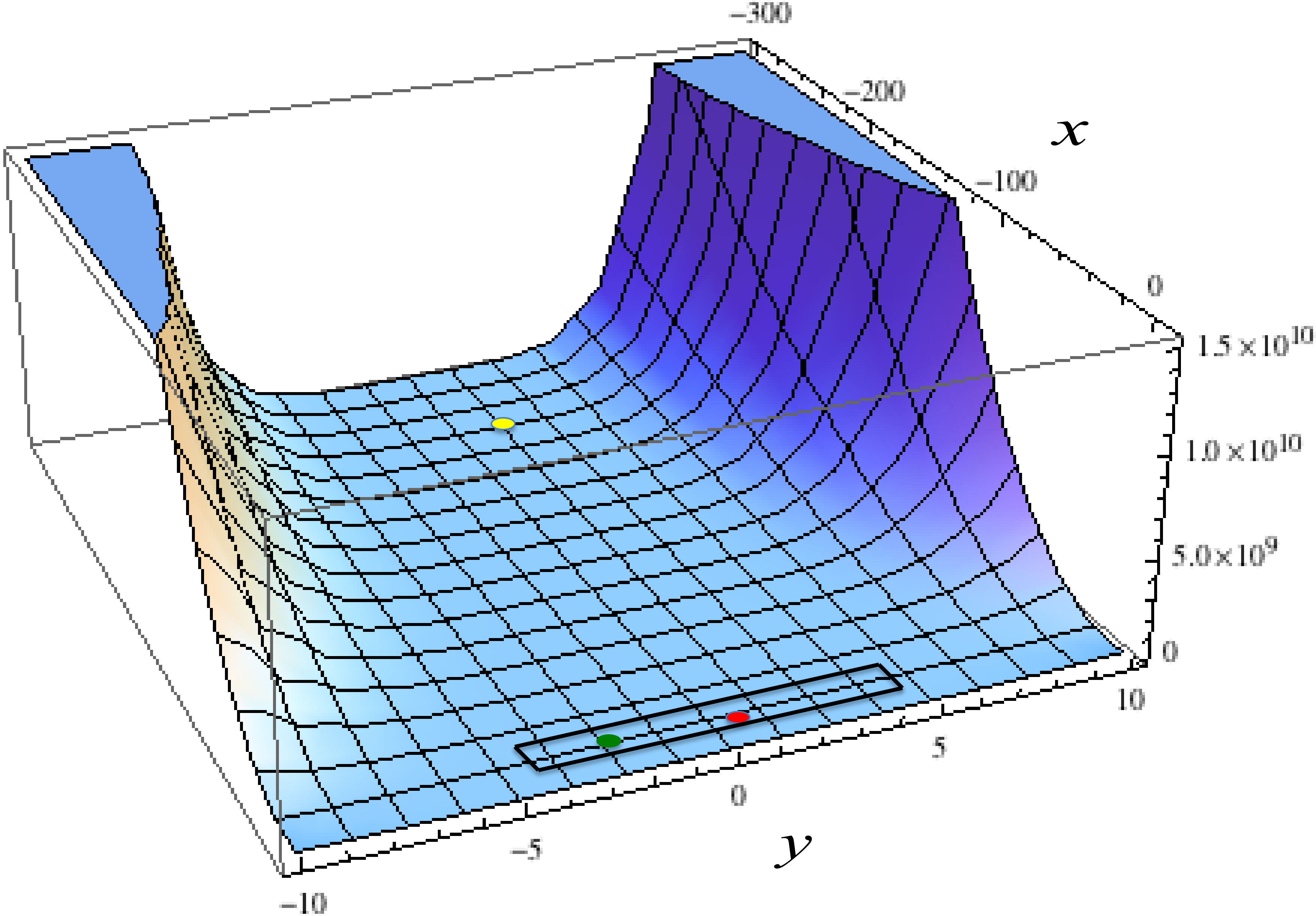
$$\text{Higher dimensional form : } f(x) = \sum_{i=1}^{N-1} [(1-x_i)^2 + A(x_{i+1} - x_i^2)^2] \; \forall x \in R^N$$


2500
2000
1500
1000
500
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
y
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
x

Performance of the LM Algorithm on the Rosenbrock Function

Dimension	Success Rate	Av. Jacobian Evals.
2	0.965	13.4
3	0.993	29.3
4	0.764	43.6
5	0.826	19.6
6	0.825	23.7
7	0.871	24.5
8	0.845	22.6
9	0.844	24.3
10	0.862	28.1

Beale : $f(x) = (1.5 - x_1 + x_1 x_2)^2 + (2.5 - x_1 + x_1 x_2^{\ 2})^2 + (2.625 - x_1 + x_1 x_2^{\ 3})^2$

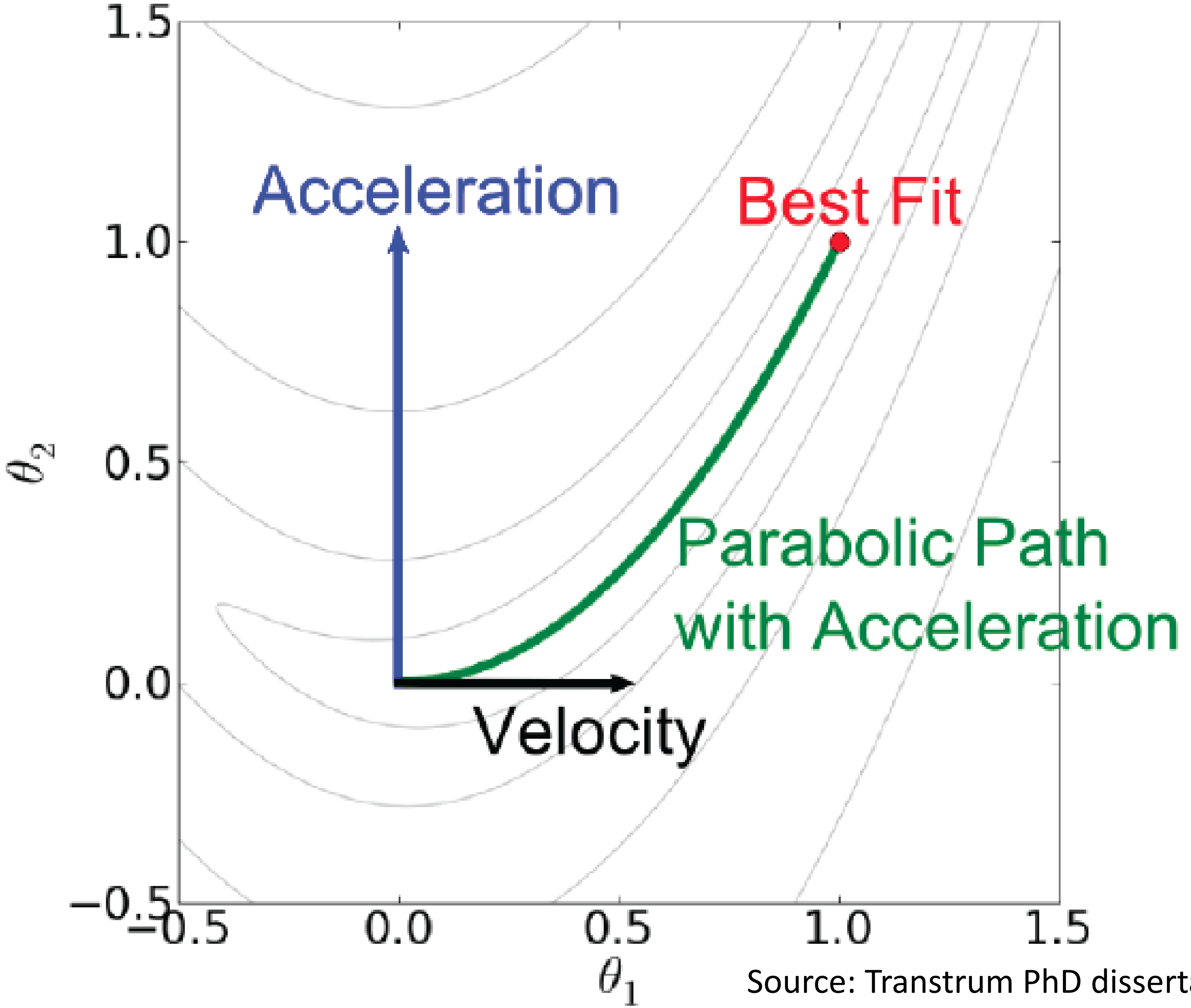


Geodesic Acceleration

- Suggested by Transtrum, Machta, Sethna (2011) as a further improvement to the LM algorithm.
- Second order correction to step – proposed step represents a truncated Taylor series:

$$\delta\theta = \dot{\theta}\delta\tau + \frac{1}{2}\ddot{\theta}\delta\tau^2$$

- In order to accept a step with acceleration added, need $\frac{|\ddot{\theta}|\delta\tau}{|\dot{\theta}|} < \alpha,$ where α is of order 1.



Source: Transtrum PhD dissertation

Description (pseudocode) of the LM algorithm with acceleration – from Transtrum, Machta, Sethna, 2011

1. Initialize values for the parameters, x, the Levenberg-Marquardt parameter λ, as well as λ_{up} and λ_{down} to be used to adjust the damping term, and α to control the acceleration:velocity ratio. Evaluate the residuals r and the Jacobian J at the initial parameter guess.
2. Calculate the metric, $g = J^T J + \lambda I$, and the cost gradient, $\nabla C = J^T r$, $C = \frac{1}{2} r^2$.
3. Calculate the velocity, $v = -g^{-1} \nabla C$, and the geodesic acceleration of the residuals in the direction of the velocity, $a = -g^{-1} J^T (v^\mu v^\nu \partial_\mu \partial_\nu r)$.
4. Evaluate the new residuals r_{new} at the point given by $x_{\text{new}} = x + v + \frac{1}{2} a$, and calculate the cost at the new point, $C_{\text{new}} = \frac{1}{2} r_{\text{new}}^2$.
5. If $C_{\text{new}} < C$ and $|a|/|v| < \alpha$, accept the step, $x = x_{\text{new}}$, and set $r = r_{\text{new}}$ and $\lambda = \lambda / \lambda_{\text{down}}$. Otherwise, reject the step, keep the old parameter guess x and the old residuals r, and adjust $\lambda = \lambda \times \lambda_{\text{up}}$.
6. Check for convergence. If the method has converged, return x as the best-fit parameters. If the method has not yet converged but the step was accepted, evaluate the Jacobian J at the new parameter values. Go to step 2.

Computation of Geodesic Acceleration

- Analytic version – directional second derivative of the residuals in the direction of the velocity.
- Finite difference estimation – two additional

function evals:

$$A_{m\mu\nu}\dot{\theta}^{\mu}\dot{\theta}^{\nu} \approx \frac{r_m(\theta + h\dot{\theta}) - 2r_m(\theta) + r_m(\theta - h\dot{\theta})}{h^2}$$

Solve $(J^T J + \lambda I)a = J^T A_{m\mu\nu}\,\theta^{\mu}\,\theta^{\nu}$ for a.

Modified Rosenbrock Function

- Used to demonstrate effectiveness of adding acceleration to algorithm.
- Residuals given by: $x,\ A(y - x^n)\ \ (n \geq 2)$

$$\text{Function}: f(x,y) = x^2 + A^2(y - x^n)^2$$

A and n control narrowness of the canyon – as A and n increase, canyon narrows. Global minimum at (0,0).

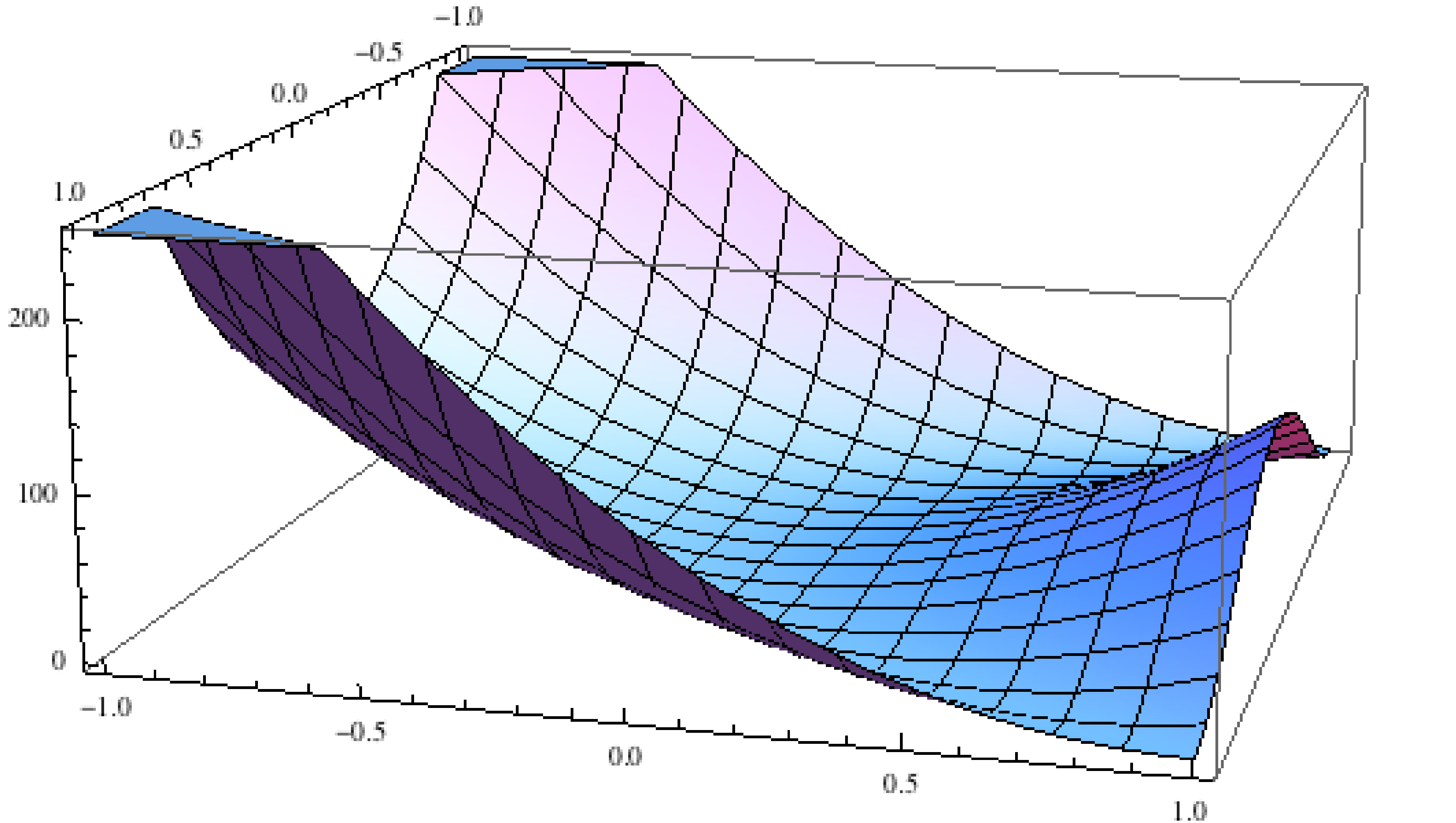
Modified Rosenbrock Tests

- Tested function with 4 different “complexities”:

1. A = 10, n = 2
2. A = 100, n = 3
3. A = 1000, n = 4
4. A = 1000, n = 5

Initial Guess: (1,1)   Convergence criteria: OF < 1e-12

- Comparison between non-acceleration and acceleration versions of algorithm (both with delayed gratification technique for updating λ).



−1.0
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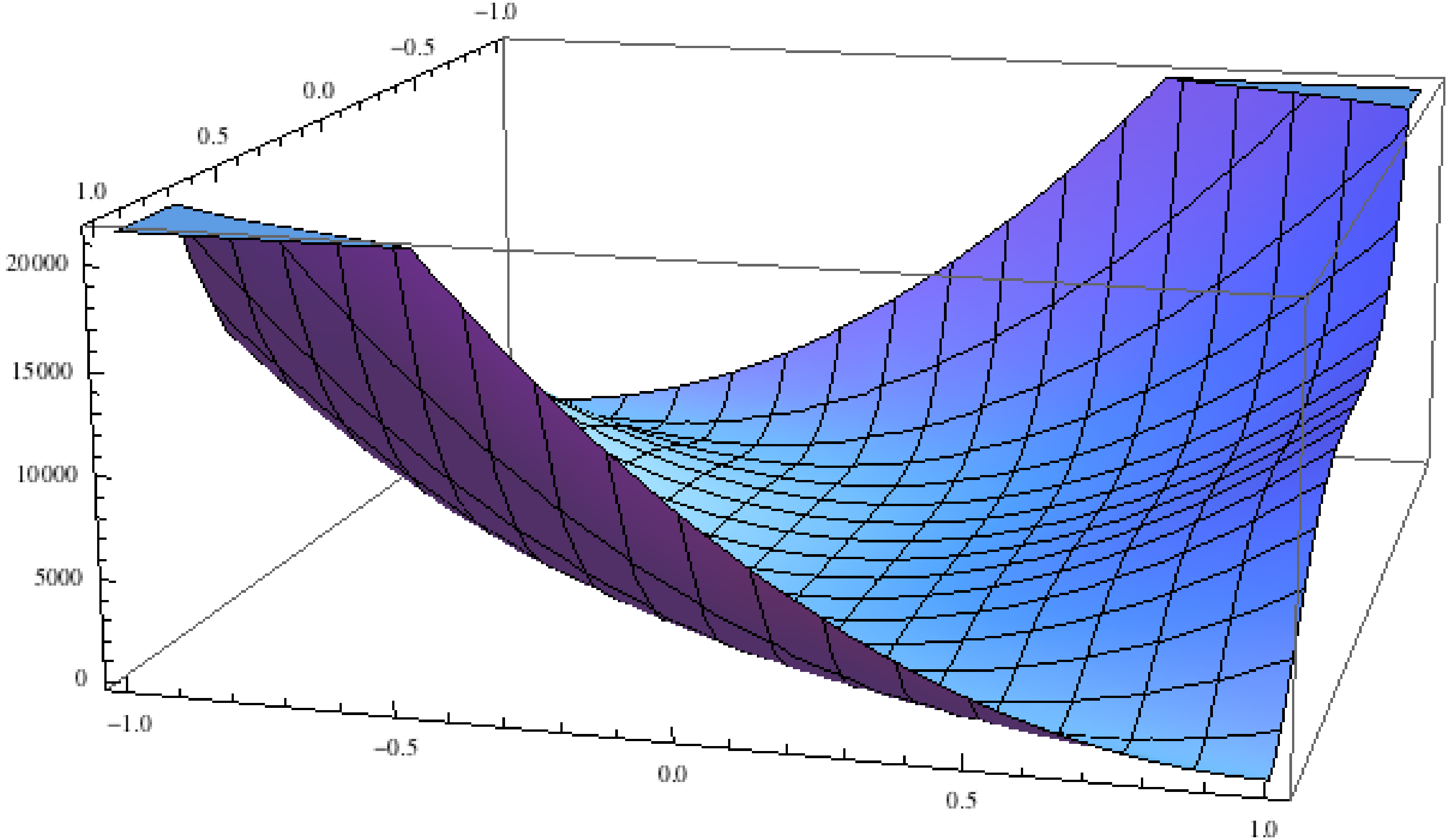
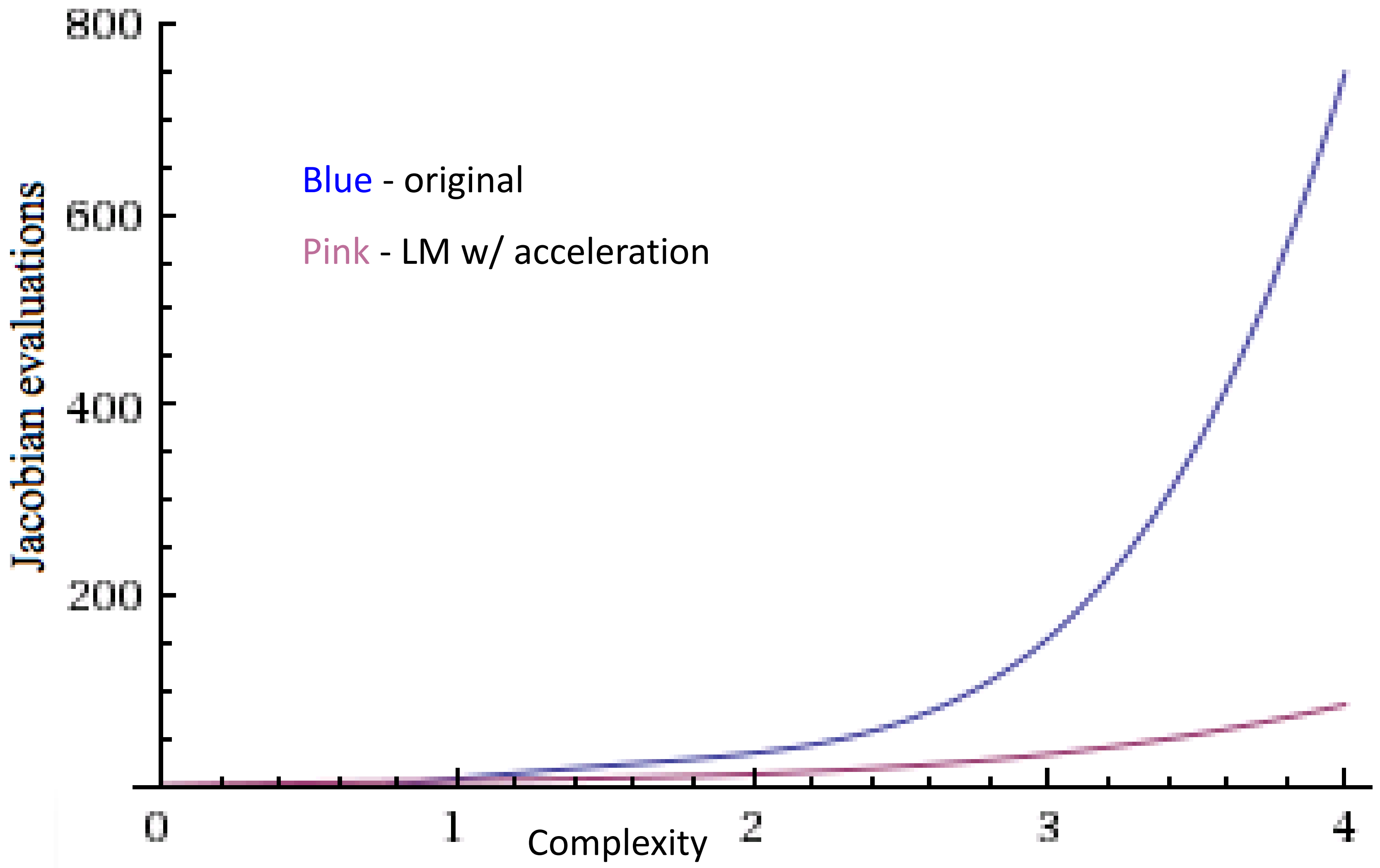
0.5
1.0
200
100
0
−1.0
−0.5
0.0
0.5
1.0



-1.0
-0.5
0.0
0.5
1.0
20000
15000
10000
5000
0
-1.0
-0.5
0.0
0.5
1.0

Original LM vs LM w/ accel for Modified Rosenbrock



Test functions

Rosenbrock : $f(x) = (1 - x_1)^2 + 100(x_2 - x_1)^2$

- Global minimum at (1, 1) - no local minima

Powell's Quadratic : $f(x) = 121x_1^2 + 5(x_3 - x_4)^2 + (x_2 - 2x_3)^4 + 10(x_1 - x_4)^4$

- Global minimum at (0, 0, 0, 0) - no local minima

Beale : $f(x) = (1.5 - x_1 + x_1 x_2)^2 + (2.5 - x_1 + x_1 x_2^2)^2 + (2.625 - x_1 + x_1 x_2^3)^2$

- Global minimum at (3.025, 0.474) - several local minima

Parsopoulos : $f(x) = (\cos x_1)^2 + (\sin x_2)^2$

- Many local minima with same minimum value

De Jong : $f(x) = x_1^4 + 2x_2^4 -$ global min. (0, 0), no local minima

Clerc's f1 : $f(x) = |x_1 \sin x_1 + 0.1x_1| + |x_2 \sin x_2 + 0.1x_2|$

- Global minimum at (0, 0), many local minima

Tripod : $f(x) = |x_1| + |x_2 + 50|$ if $x_2 < 0$, $1 + |x_1 + 50| + |x_2 - 50|$ if $x_1 < 0$,

$2 + |x_1 - 50| + |x_2 - 50|$ otherwise. Global minimum at (0, -50)

Exponential Data Fitting I - from Minpack - 2 test problem collection

$f_i(x) = y_i - (x_1 + x_2 \exp(-t_i x_4) + x_3 \exp(-t_i x_5))$ $\qquad t_i = (i-1)/10$

5 parameters, 33 residuals

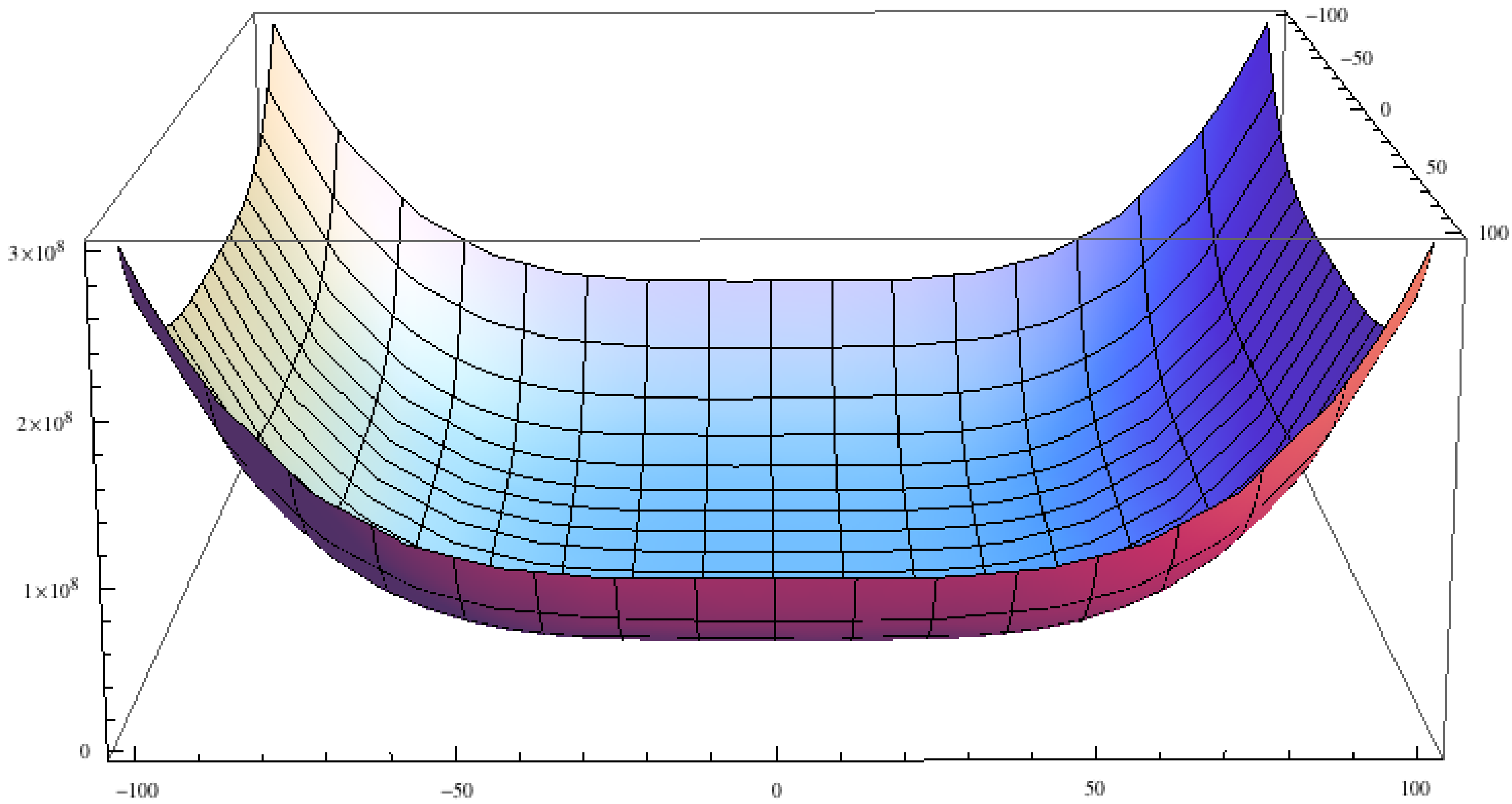
Exponential Data Fitting II - from Minpack - 2 test problem collection

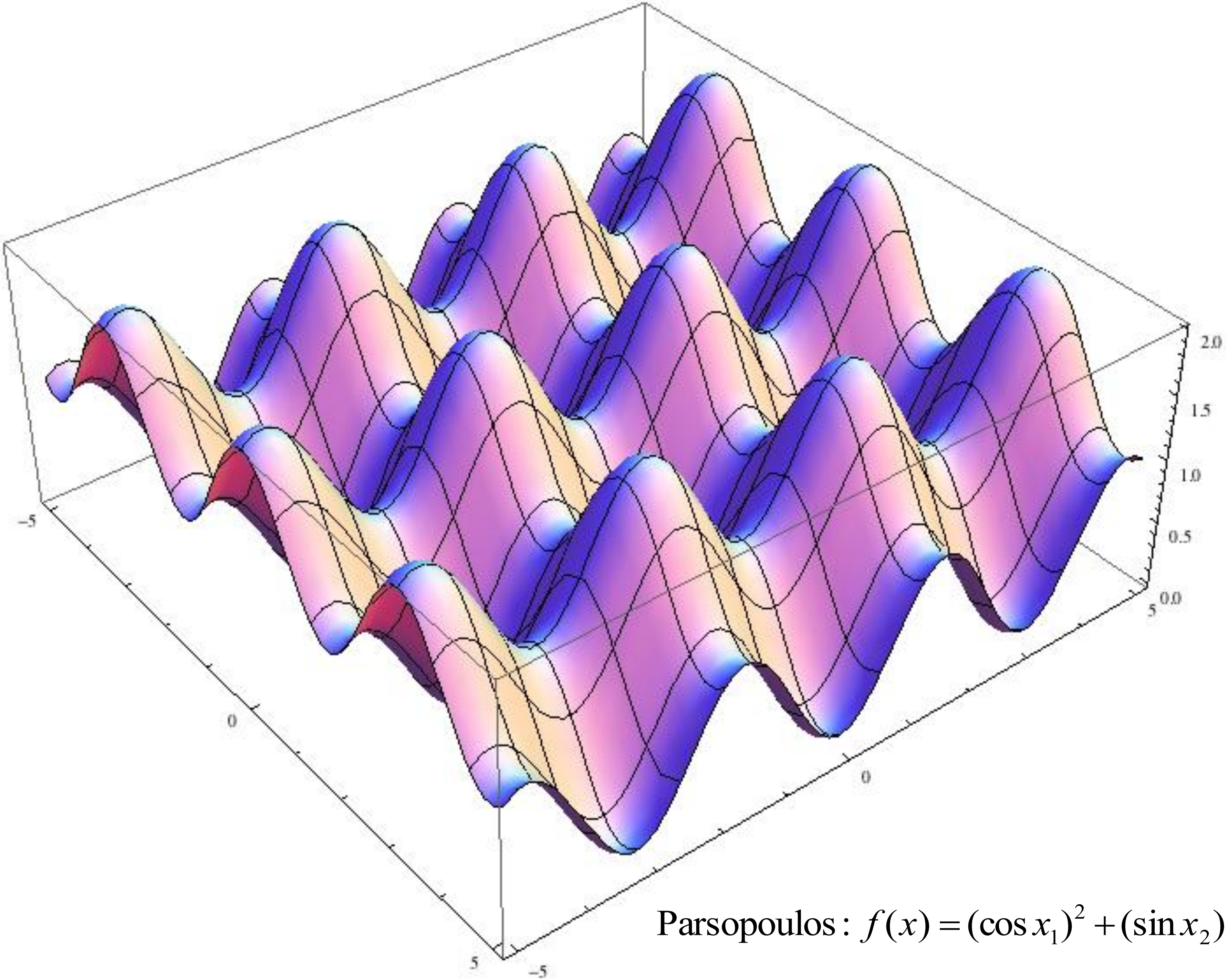
$f_i(x) = y_i - (x_1 \exp(-t_i x_5) + x_2 \exp(-(t_i - x_9)^2 x_6) + x_3 \exp(-(t_i - x_{10})^2 x_7) + x_4 \exp(-t_i - x_{11})^2 x_8))$

$t_i = (i-1)/10$ $\qquad$ 11 parameters, 65 residuals

Function	Success Rate (Original Version)	Success Rate (Accel Version)	Average Jac. Evals. (Original Version)	Average Jac. Evals (Accel Version)
2-D Tripod	0.0	0.488	1535	11.0
2-D Clerc's F1	0.896	0.909	506	4.7
Beale	0.518	0.514	19.4	12.0
De Jong	1.0	1.0	9.7	6.9
Powell's Quadratic	0.792	0.810	10.9	8.4
Parsopoulos	1.0	0.994	3.6	4.0
Exponential Data Fitting I	0.154	0.068	37.4	17.6
Exponential Data Fitting II	0.006	0.009	74.4	87.5
2-D Rosenbrock	0.965	0.936	13.3	29.8

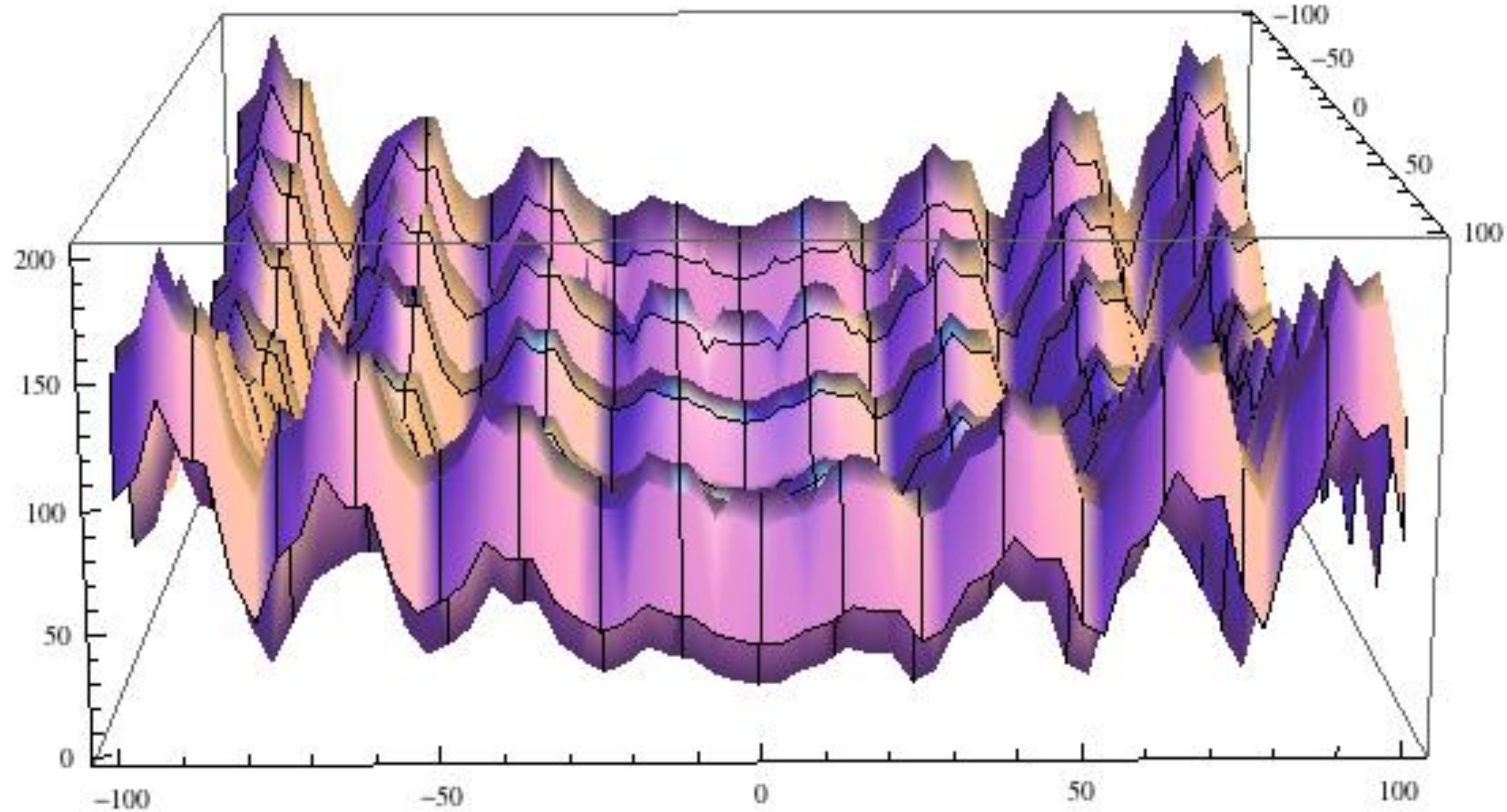
$$\text{De Jong}: f(x) = x_1^{\ 4} + 2x_2^{\ 4}$$





Parsopoulos: $f(x) = (\cos x_1)^2 + (\sin x_2)^2$

Clerc's f1: $f(x) = |x_1 \sin x_1 + 0.1 x_1| + |x_2 \sin x_2 + 0.1 x_2|$



Conclusions

- Levenberg-Marquardt algorithm is a very efficient technique for finding minima, and performs well on most test functions.
- The algorithm includes many different variables that determine its efficiency and success rate. The ideal values of these variables are very dependent on the test function.
- Implementing delayed gratification into the algorithm leads to higher success rate and fewer jacobian evaluations.
- Acceleration is an effective addition, but only in controlled situations – performance depends greatly on initial guess. Often, delayed gratification alone is enough to ensure an efficient and reliable fit, but for certain problems, acceleration can help a great deal.
- Proposed LM improvements and applied test functions are implemented in MADS (http://mads.lanl.gov)